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COMMISSION OF THE EUROPEAN COMMUNITIES

TIMOC 72 CODE MANUAL

by

R. JAARSMA and H. RIEF

1973

Joint Nuclear Research Centre
Ispra Establishment - Italy

Nuclear Study

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September 1973

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TIMOC 72 is a Monte Carlo Code for the solution of the energy and time dependent (or stationary) neutron transport equation in 3-dimensional geometries. It is an improved version of TIMOC (H. Kschwendt and H. Rief: TIMOC, A general purpose Monte Carlo code for stationary and time dependent neutron transport, EUR 4519.e, 1970) which is now written in FORTRAN IV IBM-system 360/370. Most of the features described in EUR 4519.e are also incorporated in TIMOC 72. At present it uses only the very flexible 05R geometry routine, which is able to describe any body or body-combination, with surfaces of the 2nd order. A special feature allows the calculation of small perturbation effects. It is based on the method of similar flight paths and on an iteration model to approximate an adjoint weighting function as well as the possibility of splitting in the perturbed region. A "tape storage" of the characteristic parameters of neutron histories entering the perturbed region is also possible. This allows the calculation of perturbation effects for different materials without a time consuming recalculation of the whole system. In addition the TIMOC 72 code package contains the program PLOTGEOM. It generates the data for a graphical display of cross sections of the specified geometry by the CALCOMP plotter.

KEYWORDS

T-CODES
MONTE CARLO METHOD
NEUTRON TRANSPORT THEORY
THREE-DIMENSIONAL CALCULATIONS
PERTURBATION THEORY
P-CODES
PLOTTERS
CROSS SECTIONS
MANUAL

Table of Contents

1. INTRODUCTION *)

This is a report of the FORTRAN IV version of TIMOC ("TIMOC, A General purpose Monte Carlo code for stationary and time dependent neutron transport", by H. Kschwendt and H. Rief, EUR 4519e, 1970) originally written in FAP for use on the IBM 7090/94.

TIMOC 72, as this version is called, uses an improved procedure to calculate small effects. It is based on an iteration model and the possibility of splitting in the "perturbed region". In addition, a different calculational scheme makes small effect calculations less time consuming than previously. It will be published elsewhere.

Contrary to the old version, TIMOC 72 uses only the general O5R geometry routine.

This report deals with the new input description and two sample cases. The cross section input of the Nuclear Data Preparation Program remains unchanged, but the specification of the isotope mixtures was simplified. For all other information the reader should refer to EUR 4519e. The changes in output are self-explanatory, except those dealing with ~~the~~ transmission quantities. They are explained in 5.4.1.

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*) Manuscript received on May 28, 1973

2. COMPUTER REQUIREMENTS

TIMOC is a Fortran IV program (IBM system 360) with the exception of the random number routines. They are a slightly modified version of the O5R package written in the assembler language.

The length of the program depends to a certain extend upon the compiler option used. The FTH,Ø = 2 compiler generates a program of 172 K bytes to which the length of the two data vectors DV(N) and COMM(M) has to be added. (Attention: the routine RWSAPR has to be compiled with FTG, since the FTH,O = 2 assembly contains an error). These two linear vectors contain most of the nuclear data input, the geometry input and the sampling values. This length is specified in the main program only. In the present version of TIMOC the dimensions are DV(20000) and COMM(10000). The actually required space of the data vectors is part of the print out. Since COMM(M) is only used during the Data Preparation phase (NDP-step), DV can in the next step (RWS) be extended into COMM. The available space for DV is therefore DV(N+M). Any overflow of DV or COMM is signalized.

3. PROGRAM ORGANIZATION AND DATA HANDLING

A complete computer run of TIMOC 72 consists of two or more steps. The selection of a step is ruled by certain characters on the title cards (COMCA(16), COMCA(17)). In general, the first step will be the Nuclear Data Preparation performed by the NDP program. The next step is then the execution of the Random Walk and Sampling (RWS) program.

The RWS program allows the use of several options, described in the next chapter.

If Small Effects are calculated, i.e. if the SMEC option is used, all neutron parameters, on the moment of entering into the perturbed regions, are stored in a data set with the Fortran reference number 11. On Data set 10 a basic RWS step is completed by writing a Rerun File. This file can in a RWS-RERUN step be used to augment the number of histories if an improved statistic is desired.

In the case of Small Effect Calculations in a RWS-SMEC step the Rerun file on Data set 10 serves together with the SMEC-File on Data set 11 as input and source.

4. THE NUCLEAR DATA PREPARATION PROGRAM (1st link)

The Nuclear Data Preparation Program (NDP) searches in the designated library data set for the required isotopes and prepares the macroscopic group cross sections, angular distributions, transfer matrices, etc. required for the Random Walk Sampling problem to be executed afterwards. The results of this step are written in the data vector DV(J) of blank COMMON and into the different variables of COMMON/NDRWS/. The NDP program can be in the computer simultaneously with the RWS program or as the 1st link of a chain job.

Practical remark: In many cases it is desirable to store the isotope libraries (i.e.: the microscopic group averaged cross sections usually prepared by the CODAC code) on a data set (tape) other than the Monitor input data set (5).

4.1 Input Parameters for the 1st Link Job (NDP)

CARD	COLUMNS	FORMAT	SYMBOL
1	1 - 60	15A4	COMCA(N) = 1,15

COMCA(N), N = 1,15: contains the Title identifying the job.

61	1A1	COMCA(16)

COMCA(16) must contain N (or NDP)

67	1A1	COMCA(17)

COMCA(17) is either blank if a new problem is treated or COMCA(17) is N (or NEWSMEC) if in a perturbed region nuclear data are changed for a Small Effect Calculation.

CARD	COLUMNS	FORMAT	SYMBOL
2	1 - 6	I6	DATSET
	7 - 12	I6	ADDATA
	13 - 18	I6	INPR

DATSET: Number of Data set containing the cross section libraries and nuclear parameters of the different isotopes.
If DATSET = 5: the cross sections have to be read from the Monitor input data set no. 5, i.e. they follow on cards behind card no. 2.

ADDATA: Allows the input of cross sections on data set 5 in addition to the ones on the data set specified by DATSET.
IF ADDATA $\neq$ 0: the cross sections and nuclear parameters following card no. 2 are used in addition to the ones on data set No. DATSET. If two isotop identifications are identical on data set 5 and DATSET the data on 5 have priority.

INPR: Controls the print out of the cross sections of the specified library.
If INPR $\neq$ 0: all microscopic cross sections and nuclear parameters taken from the library file and used in this computer run are printed.
If INPR = 0: no print out of these data occurs, except for the 3 comment cards (TEXT) preceeding the data of each isotope.
If ADDATA = 0 and DATSET = 5: the following cards 3 to 13 are part of the regular input on Data Set 5.

CARD	COLUMNS	FORMAT	SYMBOL

If ADDATA = 0 and DATSET ≠ 5: the following cards 3 to 13 are taken from Data Set No. DATSET (Library Tape).

If ADDATA ≠ 0 and DATSET ≠ 5: cards 3 and 4 are taken from Data Set 11 and the cards 5 to 13 of Data Set 5 are taken in addition to the ones of the Library Data Set.

3	1 - 6	I6	IM

IM: Number of energy groups, not limited.

4	1 - 11	E11.4	ENE(I): = 1, IM + 1. One card for each number.

ENE(I): The lower energy limits (in eV) of the IM energy groups in increasing order. ENE(IM+1) = upper limit of the top group. Note that the boundaries have to be the same for all isotopes. The above set of cards is required once. The following cards 5) to 13) have to be repeated for each isotope.

All the following nuclear data and group averaged cross sections can be obtained from the ENDF/B data file in the required Formats by the use of the CODAC code (Ref. 26).

Block I: Parameters which are independent of the energy-group structure

5	1 - 6	A6	ISOT Isotope identification
6	3(1-72)	3(12A6)	TEXT

TEXT: three cards, which contain a description of this isotope (origin of the cross sections, etc.; the cards may also be left blank).

CARD	COLUMNS	FORMAT	SYMBOL
7	1 - 6	A6	ISOT
	7 - 17	E11.4	ATW
	18 - 23	I6	IMF
	24 - 34	E11.4	FNY
	35 - 45	E11.4	AFIS
	46 - 56	E11.4	BFIS
	57 - 67	E11.4	CFIS

ISOT: Isotope identification

ATW: Atomic weight of the isotope

IMF: Number of different fission spectrum representations to be used (≤ 3)

The energy dependence of the number ν of secondary fission neutrons is assumed to be described by the following polynomial fitting:

$$\nu(E) = FNY + AFIS*E + BFIS*E^2 + CFIS*E^3$$

E = energy (eV).

$\nu(E)$ can also be given as a group averaged value for each energy group separately, see card 9.

8	1 - 6	I6	LTT
	7 - 17	E11.4	EMIN
	18 - 28	E11.4	EMAX
	29 - 39	E11.4	ELCO(1)
	40 - 50	E11.4	ELCO(2)
	51 - 61	E11.4	ELCO(3)

LTT: Symbol defining type of fission spectrum

EMIN, EMAY: Lower and upper limit (in eV) for the corresponding fission spectrum

CARD	COLUMNS	FORMAT	SYMBOL

ELCO(1): A

ELCO(2): B

ELCO(3): C

LTT = 6 or 7: Simple fission spectrum

$$\chi(E) = B\sqrt{E}\,\exp(-E/A)$$

LTT = 8 or 9: Maxwellian distribution

$$\chi(E) = B \cdot E \cdot \exp(-E/A)$$

LTT = 10: Watt spectrum

$$\chi(E) = C \cdot \exp(-E/A) \cdot \sinh(\sqrt{B \cdot E})$$

There can be a maximum of 3 cards of type 8 per isotope.

Block II: All microscopic group averaged cross sections split into the capture, elastic scattering, inelastic scattering and fission parts and (optional) the particle multiplication factor for fission.

9	1 - 6	A6	ISOT
	7 - 17	E11.4	ENCH
	18 - 28	E11.4	CROM(1)
	29 - 39	E11.4	CROM(2)
	40 - 50	E11.4	CROM(3)
	51 - 61	E11.4	CROM(4)
	62 - 72	E11.4	CROM(5)

ISOT: Isotope identification

ENCH: Lower boundary of the energy group (eV)

CARD COLUMNS FORMAT SYMBOL

CROM(1): is σ_{CA}, the microscopic capture cross section
Unit: barn (= 10^{-24} cm^2).

CROM(2): is σ_{EL}, the microscopic elastic scattering cross section
Unit: barn.

CROM(3): is σ_{IN}, the microscopic inelastic scattering cross section
Unit: barn.

CROM(4): is σ_{FI}, the microscopic fission cross section
Unit: barn.

CROM(5): is ν (like on card 7). If CROM(5) $\neq$ 0, this value is taken for the determination of the product $\nu\sigma_{FI}$.

Block III: All information on elastic isotropic or anisotropic scattering

A card 10 must be present for each energy group (in increasing order) in which $\sigma_{EL} \neq 0$. If required, card 10 must be followed by the corresponding card 11. The card(s) describe(s) the differential cross sections for the elastic anisotropic scattering.

10	1 - 6	A6	ISOT
	7 - 17	E11.4	ENCH
	18 - 23	I6	LTT
	24 - 29	I6	NE

ISOT: Isotope identification

ENCH: Lower boundary of the energy group (eV)

LTT: Symbol defining angular distribution description

NE: Number of parameters following on card 11

CARD	COLUMNS	FORMAT	SYMBOL

LTT = -1: The same angular distribution function as in the previous group is used. Card 11 must be omitted.

LTT = 0: Isotropic scattering distribution in the c.m. system. Card 11 must be omitted.

LTT = 1: The distribution is described by a Legendre polynomial in the c.m. system. The program expects on card 11 NE Legendre coefficients for the anisotropic distribution.

$$\frac{d\sigma}{d(\cos\vartheta)} = \sum_{n=0}^{NE-1} ELCO(n+1)\cdot P_n(\cos\vartheta).$$

LTT = 2: Anisotropic scattering is described in the c.m. system by a polygon. NE is the number of equidistant points along the μ-axis in the $d\sigma/d\mu$ table (≤ 40).

LTT = 3: The averaged value cos Θ of the angular distribution in the lab. system is used.

Card(s) 11 must only be given, if LTT $\geq$ 1.

11	1 - 11	E11.4	ELCO(1)	
	.	.	.	ELCO(I),I = 1,NE
	.	.	.	
	.	.	.	
	56 - 66	E11.4	ELCO(6)	
	etc.			

If LTT = 1: The ELCO(I) are the NE coefficients of the Legendre polynomial.

CARD	COLUMNS	FORMAT	SYMBOL

If LTT = 2: The ELCO(I) are the NE values ($\leq$ 40) of the angular distribution $d\sigma/d\mu$ at equidistant points between $[+1, -1]$, including the boundaries. The number of intervals is therefore NE-1. The ELCO(I) must be given for the distribution in the c.m. system and in decreasing order of $\cos\vartheta$ $[+1 \rightarrow -1]$.

Note that in each group another type of anisotropic scattering may be used.

Block IV: All information on inelastic scattering and transfer matrices

12	1 - 6	A6	ISOT
	7 - 17	E11.4	ENCH
	18 - 23	I6	LTT
	24 - 29	I6	NU

ISOT: Isotope identification

LTT defines the inelastic scattering description

ENCH: Lower energy boundary

NU: Number of parameters following on card 13

LTT = -1: The same scattering values are used as in the previous energy group.

LTT = 1: The model of excited levels is used.

LTT = 2: The statistical model is used.

LTT = 3: Energy transfer is described by a transfer matrix.

Card 13 must be given if LTT $\geq$ 1.

If LTT = 1 or 2 card 13 reads like

13	1 - 11	E11.4	ELCO(1)	
	.	.	.	
	.	.	.	ELCO(1),I = 1,NU
	.	.	.	
	56 - 66	E11.4	ELCO(6)	

a) For LTT = 1 and NU $\geq$ 2 (excited level description) this means:

ELCO(1): Δ E for first energy level (Δ E is negative for down scattering)

ELCO(2): Partial probability for first level

ELCO(3): Δ E for second level and so on until NU values have been read in. The partial probabilities are normalized by the program and the sum does not have to agree with the total inelastic cross section.

Since in most calculations discrete energy values appear during the course of a history it can happen that in some energy group the subtraction of Δ E leads to a negative value of the energy after the collision. If $E - \Delta E < 0$, for $E_{i+1} < E \leq E_i$, the program chooses another level (if possible) or an elastic collision process. In the case where a partial cross section for level excitation does not exist over the whole range of a group, it should only be averaged over the range where it is different from zero:

CARD	COLUMNS	FORMAT	SYMBOL

b) For LTT = 2 and NU = 1 (statistical model (ELCO(1)) is the nuclear temperature for the group under consideration.

c) If LTT = 3 and NU $\geq$ 3 (transfer matrix version in this energy group)

13	1 - 6	I6	
	7 - 17	E11.4	
	18 - 28	E11.4	
	29 - 34	I6	ELCO(I),I = 1,NU
	35 - 45	E11.4	
	46 - 56	E11.4	

ELCO(1): is the number of energy groups which the neutron skips after the collision

ELCO(1) = 0: scattering into the same energy group

ELCO(1) = -0: only down scattering in the same group

ELCO)1) = +m (-m): up (down) scattering into a group defined by adding (subtracting) m to (from) the actual energy group index

ELCO(2): relative probability for the particle to jump into the energy group specified by ELCO(1)

ELCO(3) = averaged value of the angular distribution (cos Θ) in the lab. system for the corresponding scattering process.

ELCO(4): like ELCO(1) and so on.

Usually the sum of the ELCO(2) + ELCO(5) + ... coincides with the corresponding value of σ_{IN} on card 9.

If this is not the case, i.e. if $\sigma_{IN} \neq \sum$ ELCOT(2+3j), the ratio ELCO(2+3j)/σ_{IN} is calculated, and during the execution of the Monte Carlo calculations the neutron weight after an inelastic collision is multiplied each time by this factor. This feature can, for example, be used to describe particle multiplication processes such as the (n,2n) reaction. For further details see the above paragraph dealing with transfer matrix calculations.

Note that in each energy group another type of inelastic scattering may be used.

Cards 5 to 13 have to be repeated for the next isotope.

If ADDATA ≠ o or DATSET = 5 there follows a card 14 with ISOTX(N) = END after the parameters of the last isotope.

CARD	COLUMNS	FORMAT	SYMBOL
14	1 - 6	A6	ISOTX(KX)

ISOTX(KX) = END

15	1 - 6	I6	MM: number of mixtures ($\leq$ 50)
	7 - 12	I6	LM: number of different geometrical regions ($\leq$50), LM $\geq$ MM)
			In the O5R geometry the meaning of LM becomes that of the so-called "material regions". See Input description of the O5R geometry.

CARD	COLUMNS	FORMAT	SYMBOL
16	1 - 6	I6	MIXTC: mixture number, in the order 1,2,...M
	7 - 12	I6	NM: number of isotopes in this mixture NM $\leq$ KM
17	1 - 6	A6	ISOT(1)
	7 - 18	E12.5	CRO(1)
	.	.	. ISOT(I), CRO(I) = 1,NM
	.	.	.
	.	.	.
	55 - 60	A6	ISOT(4)
	61 - 72	E12.5	CRO(4)

This card specifies the isotope concentration in the different mixtures.

ISOT(I): isotope identification

CRO(I): nuclear density of the isotope (number of atoms in units of 10^{24} per cm^3)

For each mixture, a pair of card 16 and card(s) 17 is required.

18	1 - 6	I6	LCH: region number in increasing order 1,2,3,.... LM

This card correlates geometrical region and mixture number.

7 - 12	I6	JRGN(I): number of the mixture filling this region. There must be a card 18 for each region.

Parameters for the fission spectrum of the primary neutrons:

CARD	COLUMNS	FORMAT	SYMBOL
19	1 - 6	I6	IFM: number of different fission spectrum representations to be used (≤ 3)
20	1 - 6	I6	LTT: symbol defining type of fission (spectrum description in 9.1.1, Block I)
	7 - 28	2E11.4	EMIN, EMAX: lower energy limit of the corresponding fission spectrum in eV.
	29 - 61	3E11.4	A,B,C: coefficients of the different fission spectra described in 9.1.1, Block II ($C \neq 0$ only for LTT = 10)

4.2 The Nuclear Data Output

The NDP program writes the following output:

The job title

The list of isotope specifications and the numbers assigned to them:

ISOTOPE NO.(I2) = (6a)

A list of all mixtures and their isotope composition:

MIXT. No. (I2)

(A6) - DENS. = (EI2.5), (A6) - DENS. = (E12.5),....

A list correlating the region number with its mixture number:

RG(I2) MIXT. NO. (I2)

The paramters of the fission spectra of the primary or source neutrons:

FISS. SPECT. PARAMETERS FOR PRIM. NEUTRONS

FISS. SPECT. * TYOE NO. (I6), FROM E = (E11.4) TO (E11.4) EV, PARAM. S=(3E11.4)

5. THE "RANDOM WALK SAMPLING" PROGRAM (2nd link)

5.1 Operational Modes and Options (specifications)

As already mentioned above, the TIMOC code can be operated in different modes (e.g. Initial values problems = Standard Version, Eigenvalue problems = ITER ★ option etc.). In addition, different sampling procedures can be applied and a number of quantities calculated optionally. In what follows, the various operational methods and specifications are listed in alphabetical order:

ANGL ★ : The direction of the flight vector of the external source neutrons (primary neutrons) is fixed and has to be specified in card 4.

CLLD ★ : The distribution function of the number of collision is sampled.

DUMP ★ : Gives a dump of all interesting quantities at each collision and each boundary crossing.

ELP ★ : The "Expected Leakage Probability" version of TIMOC is executed. In addition (see EUR 4519) LEAK ★ must be specified. (not yet valid)

EMIN ★ : Specifies a lower energy limit which is higher than the lower energy limit of the cross sections in use (card 4).

ENDE ★ : The energy depositions due to elastic scattering is sampled.

FLUX ★ : Region and energy dependent fluxes are calculated by the track length estimator.

GRVE ★ : To each energy interval an average group velocity is assigned. This group velocity is used for calculations of the time parameters instead of the discrete velocities obtained from discrete neutron energies.

ITER ★ : Specifies an eigenvalue calculation where in a multiplying medium successive neutron populations are generated. The sample values are taken from this iteration process under the assumption that the fundamental mode distribution has been reached (see Sec. 6.2).

LEAK ★ : Specifies a geometrical region as a leakage zone; i.e. neutrons entering this region are terminated. The leakage region has to be specified in the geometry input by 0.

MTIM ★ : The mean lifetime for leakage, absorption and slowing down, the mean generation time for each fissionable isotope and the mean scattering time are sampled.

RURU ★ : The Russian Roulette version is used (Sec. 4.2., EUR 4519)

SMEC ★ : Allows the calculation of differential effects which are smaller than the variance of the sampled quantity itself.
The so-called perturbed regions have to be specified in card 4.

STEN ★ : The source or primary neutrons start with a fixed energy. Card 7 must be specified.

TIME ★ : The time dependent solution is desired. At each collision and crossing point all necessary parameters are written on the Time Tape. Not yet published.

TMAX ★ : Neutron histories are only followed in the time range $0 \leq t \leq$ TMAX ★ . Together with the ELP ★ version this is a powerful variance reducing procedure if time dependent problems are treated (see EUR 4519 and Ref. (10)).

TRAN ★ : Transmission quantities (flux, current and first angular moment of the current) are sampled at specified region interfaces. See LTRM and LLTR1(LTR) and LLTR2(LTR) of the NAMLIST INPUT and App. D.

VARC ★ : Makes it possible to calculate the probable error of the flux for a specified energy group and region.

5.2 Input Data and Formats

CARD	COLUMNS	FORMAT	SYMBOL
1	1 - 60	15A4	COMCA(N), N = 1,15 COMCA(N): Title card to identify the job. It must agree with card 2 of the NDP input data.
	61	1A4	COMCA(16)
	COMCA(16) must be R (or RWS)		
	67	1A4	COMCA(17)

CARD	COLUMNS	FORMAT	SYMBOL
			COMCA(17) is blank if a new problem is treated or COMCA(17) is S (or SMEC) if a Small Effect Calculation is performed for the nuclear data composition specified in the NDP-Link of the program. Or COMCA(17) is N (or NEWSMEC) if a Small Effect Calculation is performed for a new nuclear data composition in the perturbed region. (In this case cards 2 to 4 have to be repeated). Or COMCA(17) is R (or RERUN) if the Rerun Procedure is used, which allows the continuation of the problem at a later time. In all cases where COMCA(17) is S or R card 1 is followed only by a namelist input with the NAMELIST name RERUN. (See the "Rerun Procedure", Sec. 5.3).
2	1 - 6	I6	N N: number of 6-character-words following in columns 13-72.
	7	11(A4,2X)	All specifications and options which are used in this computer run (see Sec. 5.1).
2a	7 - 72	11(A4,2X)	Continuation of card 2 (if necessary).
3	1 - 12	I12	HMAX: number of primary neutron histories to be calculated.
	13 - 24	I12	HFMAX: number of secondary neutron histories to be calculated (≥ 1). When either of these two numbers is reached the calculation is terminated and a full

CARD	COLUMNS	FORMAT	SYMBOL
			output is printed. For an eventual continuation of the problem see the "Rerun Procedure" (see Sec. 5.3).
	25 - 36	Z12	R: initial random number; if not specified, the program takes 1.
4	2 - 7		&INPUT
	9 etc.		NAMELIST NAMES as described below
			&END

The specification of input parameters (in card 4) refering to an option (e.g. LQSM = i_1, NTRM = i_2, etc.) turns the option on, even if it was not specified in card 2.

5 and all following cards describe the geometry input. See the special input description in Sec. 6 and ORNL.

The following input parameters which are all optional are read by the NAMELIST procedure of FORTRAN IV. The NAMELIST name is INPUT. The NAMELIST items are:

IGM : number of energy groups for which the energy dependent output quantities are sampled.

$$0 \leq \text{IGM} \leq 50$$

If IGM = 0 (or not specified) the program uses the group structure of the nuclear data library, i.e. the group structure specified by cards 3 and 4. In this case the condition IGM = IM $\leq$ 50 must hold.

EG(IG) : group boundaries of the energy dependent output quantities in [eV]. IG = 1,(IGM+1).

EZE : allows to change the lower energy limit independent of EG(1) or ENE(1). It is only effective if EZE > EG(1) (lower limit of the first energy group).

UVST, VVST, WVST: assigns a fixed direction vector to histories starting in the source point.

EST: assigns a fixed energy to histories starting from the source point.

NTM : number of intervals of the Time Distribution Functions. NTM $\leq$ 50. If NTM = 0 or not specified, the calculation of the time distribution functions is omitted. If NTM = 50: the program sets automatically TMAX = TDI(NTM+1).

TDI(NT): boundaries of the time distribution intervals. The quantities have to be in increasing order. TDI(NT); NT = 1, (NTM+1)

NGVM: number of group velocities. It must be equal to the number of energy groups of the nuclear data input, i.e. NGVM = IM. This option allows an average group velocity to be specified for each energy group ENE(I). If NGVM is not specified the program calculates the velocity for the discrete neutron energy E. NGVM $\leq$ 50

GRVE(I): average neutron velocity for energy group ENE(I) in [sec]. GRVE(I), I = 1,NGVM.

LVAR, IGVAR: these two specifications allow the error of the neutron flux in geometrical (or material) region L and energy group IG to be estimated.

HDPZE, HDPMX, HFDPZE, HFDPMX: allow a detailed history dump of primary (HDP..) and/or secondary (HFDP..) histories. The dump is performed from history number ...ZE to ...MX.

LQSM: total number of regions for which a Small Effect Calculation will be performed. $0 \leq$ LQSM ≤ 10

LQS(LQS): Region Numbers (L) for which the Small Effect Calculation will be performed.

HPRINT: controls the Intermediate Print Out. After each multiple of HPRINT histories the program produces an intermediate print out. If it is not specified HPRINT = 1000.

TIMPMX : the job will be completed with a Final Print Out after TIMPMX seconds have passed. At the same time all quantities necessary for a re-run are stored on Data set 10. If TIMPMX is not specified it is /10.000.

LTRM : allows the sampling of neutron Transmission quantities between two adjacent regions. LTRM is the number of areas for which such a calculation is performed. LTRM $\leq$ 20; see Appendix D.

LLTR1(LTR); LLTR2(LTR): region numbers of the two adjacent regions for which the transmission is calculated. LLTR1(LTR), LLTR2(LTR); LTR = 1,LTRM.

QRERUN : if QRERUN = FALSE, the Re-Run Procedure is canceled, i.e. no Re-Run Data Set has to be specified.

K5GEO : specifies the Data Set on which the input parameters for the geometry are stored. If it is not specified K5GEO = 5.

NSPQSM: Splitting Factor for neutron histories after entering the region(s) for which a small Effect Calculation is performed.

5.3 Application of the O5R Geometry

1) Starting point

In the following the terminology of the O5R geometry is used to describe the generation of starting points.

A starting point may be a fixed point in a sector or a random point in a sector (starting sector). Thus, a starting sector contains equally distributed starting points. A starting block is a block that contains a starting sector. The medium number (starting medium) in a starting sector must be unique in the starting block to which it belongs. The number of fixed starting points or starting sectors with an equally distributed random source or the combination of both is only limited by the available storage space. To each fixed starting point or starting block a relative probability of selection must be assigned.

The subroutine GSTRT operates as follows:

1. By means of their relative probability either a starting point or a starting block is selected.
2. If a starting block has been selected, then a point is randomly generated in this block and rejected if the medium containing this point is not the starting medium of this block.
3. In the case of rejection, step 2 is repeated, at most 1000 times. If the medium found in step 2 is equal to the starting medium the generated point is the starting point.

2) The geometry input

I. The GEOM input. See the O5R report and appendix A.2.

Only material media are considered, therefore the index of card A (in the O5R report) is 2. Medium number 1000 does not refer to internal void. Internal void (vacuum) should be defined as a medium with a density of zero, so that $\Sigma^T = 0$.

II. The description of starting points

Card S: Format ($\overset{a}{I6}$)

a - The total number of fixed starting points and of starting blocks

Card T: Format ($\overset{a}{E12.5}$,$\overset{b}{E12.5}$,$\overset{c}{E12.5}$,$\overset{d}{E12.5}$,$\overset{e}{I6}$,$\overset{f}{A6}$)

For each fixed starting point and for each starting block there is one card.

a - X - coordinate
b - X - coordinate
c - Z - coordinate
} see f

d - The relative probability given to the starting point or block (starting sector)

e - The medium number in the point (X,Y,Z)

f - blank or RANDOM. If f = blank the point (X,Y,Z) serves as starting point, if f = RANDOM points X,Y,Z are chosen at random with equal probability in the internal region e.

The medium number in e has to be given only for checking reason as the medium is already determined by the point (X,Y,Z).

5.4 The Final Output of Sample Values

The sampling procedures and output formats agree in most cases with those of TIMOC. The user of TIMOC 72 should therefore refer to EUR 4519 e, except for the transmission quantities which are described below (5.4.1).

5.4.1 The Sampling Procedure of Neutron Flux, Current and Angular Flux at Interfaces of Adjacent Regions

In TIMOC 72 the sampling procedure of neutron transmission quantities at interfaces of adjacent regions has been improved compared to the one used in TIMOC (EUR 4519 e, 1970). It is now possible to sample the flux, the current and the first angular moment of the current. These quantities inserted into a Legendre expansion allow in addition the P_2-approximation of the angular flux, which is sometimes of particular interest at free surfaces. The quantities which appear in the print out are headed by the following labels:

ENERGY GROUP, PHI(L_1 /L_2), TRO(L_1 /L_2), TRO(L_1 /L_2), PHI(L_2 /L_1), TRO(L_2 /L_1), TRO(L_2 /L_1), and TR1(L_2 /L_1)

These bivariate tables give the transmission quantities as a function of the specified energy groups and the passage from region L_1 to L_2 and viceversa. The pair correlation L_1 /L_2 corresponds to the input specification of the parameters LLTR1(1) = L_1 and LLTR2(1) = L_2 etc.

In the notation of EUR 4519 e the three sample values are defined as follows:

A) Standard Version

$$PHI(L_1/L_2)_i: \quad = \left[\sum_h \sum_g w_{h,g}(L_1/L_2,i) \Big/ \left| \mu_{h,g}(L_1/L_2,i) \right| + \right.$$

$$\left. + \sum_n \sum_g w_{h,g}(L_1/L_2,i) \Big/ \left| \mu_{n,g}(L_1/L_2,i) \right| \right] \cdot s \cdot S^{-1} F^{-1}$$

$w_{h,g}(L_1,L_2,i)$: weight of a neutron track (belonging to energy group E_i) crossing the interface from region L_1 to region L_2 .

$\mu_{h,g}(L_1/L_2,i)$: cosine of the same track vector with the surface normal of the interface.

F: area of the interface between region L_1 and L_2 . Since in the present version of the program this surface area is not calculated we set F = 1.0

s,S: normalization factors which correspond to the definition of EUR 4519.e, pag. 108-110.

The physical meaning of $PHI(L_1/L_2)$ is that of a surface flux in direction L_1 to L_2 . The total surface flux at the interface L_1/L_2 is obtained by adding $PHI(L_2/L_1)$.

$$TRO(L_1/L_2)_i = \left[\sum_h \sum_g w_{h,g}(L_1/L_2,i) + \sum_n \sum_g w_{n,g}(L_1/L_2,i) \right] \cdot s \cdot S^{-1} F^{-1}$$

i.e. the total number of neutrons crossing the interface from L_1 to L_2 and corresponds therefore to the definition of the current in this direction.

$$TR1(L_1/L_2)_i = \left[\sum_h \sum_g w_{h,g}(L_1/L_2,i) \cdot \left| \mu_{h,g}(L_1/L_2,i) \right| + \right.$$

$$\left. + \sum_n \sum_g w_{n,g}(L_1/L_2,i) \cdot \left| \mu_{n,g}(L_1/L_2,i) \right| \right] \cdot s \cdot S^{-1} \cdot F^{-1}$$

i.e., the first angular moment of the current (or the second moment of the vector flux) crossing the interface from L_1 to L_2.

The quantities $PHI(L_1/L_2)$, $TRO(L_2/L_1)$ and $TR1(L_2/L_1)$ are the transmission quantities into the opposite direction; the current $TRO(L_2/L_1)$ is for obvious reasons printed with a minus sign.

B) ITER* Version

$$PHI(L_1/L_2)_i = \left[\sum_n \sum_g w_{n,g}(L_1/L_2,i) \Big/ \left| \mu_{n,g}(L_1/L_2,i) \right| \right] \cdot (S_{IT} \cdot F)^{-1}$$

Also $TRO(L_1/L_2)$, $TR1(L_1/L_2)$ etc. are calculated by omitting the term

$$\sum_n \sum_g \cdots\cdots$$

Angular Flux at a Surface Calculation

Inserted into a Legendre expansion the three sample values PHI, TRO and TR1 can be used for the calculation of angular dependent mean flux at the surface a (transmission between L_1/L_2 and L_2/L_1) and the energy groups E_i.

$$\Phi(a,i,\mu) = \frac{1}{4\pi} \sum_{L} (2L+1) g_L(i) P_L(\mu) \qquad (1)$$

The first three polynomials are:

$$P_o = 1, \quad P_1 = \mu, \quad P_2 = \frac{1}{2}(3\mu^2 - 1)$$

and

$$\varphi_o(i) = 2\pi \int_o^1 d\mu \Phi(L_1/L_2,i,\mu) = PHI(L_1/L_2,i) + PHI(L_2/L_1,i)$$

$$\varphi_1(i) = 2\pi \int_o^1 \mu d\mu \Phi(L_1/L_2,i,\mu) = TRO(L_1/L_2,i) - TRO(L_2/L_1,i)$$

$$\varphi_2(i) = \pi \int_o^1 3\mu^2 d\mu \Phi(L_1/L_2,i,\mu) - \pi \int_o^1 d\mu \Phi(L_1/L_2,i,\mu) =$$

$$= \frac{3}{2} TR1(L_1/L_2,i) + TR1(L_2/L_1) - \frac{1}{2} PHI(L_1/L_2,i) + PHI(L_2/L_1,i)$$

Inserted into eq. (1) one obtains if PHI $(L_1/L_2,i)$ + PHI$(L_2/L_1,i)$ is set to PHI(a,i):

$$\phi(a,i,\mu) = \frac{1}{4\pi}\left\{ PHI(a,i) + 3\,TRO(a,i)\,\mu + \frac{5}{4}\left[3\,TR1(a,i) - PHI(a,i)\right](3\mu^2 - 1)\right\}$$

For the special case $\mu = 1$, i.e. the angular flux perpendicular to the surface, the (= 4π equivalent flux) $4\pi\,\phi(a,i,\mu = 1)$ is printed in a bivariate table for all energy groups.

For the purpose of control also the angular flux in a solid angle of 2 steradion is sampled around the surface normal and printed as the 4π -equivalent flux. It refers only to the transmission L_1 to L_2 and is listed in the table under the subtitle:

4*PI EQI. OF 2 STERA. AVA.

$$FL*DE(L_1/L_2) = 2\pi\left[\sum_h \sum_{g(\mu^*)} w_{h,g}\Big/|\mu_{h,g}| + \sum_n \sum_{g(\mu^*)} w_{n,g}\Big/|\mu_{n,g}|\right]\cdot s\cdot S^{-1}\cdot F^{-1}$$

$g(\mu^*)$: Summation over g only for $\mu_{h,g} > 0.682$.

The values $4\pi\,\phi(a,i,\mu = 1)$ obtained by the P_2-approximation are listed under the heading:

4* PI EQI OF P-2 APPROXI.

$$FLXDE(L_1/L_2) = PHI(a,i) + 3*TRO(a,i) + \frac{5}{2}\left[3*TR1(a,i) - PHI(a,i)\right]$$

and

$$FL(L_1/L_2) = FLXDE(L_1/L_2).$$

5.5 The ReRun Procedures

The Rerun procedure is either used to increase the number of histories or to calculate a Small Effect in one or more geometrical regions after the execution of the so-called "basic case".

5.5.1 The Rerun for Increasing the History Number

A calculation can be continued (for improving the statistics) if it has reached completion or if the specified time TIMPMX on card 4 was exceeded. In both cases a Rerun File, containing all the necessary information for continuation is stored on Data-set 10. The input for continuation consists of:

CARD	COLUMNS	FORMAT	SYMBOL
1	1 - 60	15A4	COMCA(N),N = 1,15
	COMCA(N),N = 1,15 has to agree with the title of the job being continued		
	61	1A1	COMCA(17) = R(or RWS)
	67	1A1	COMCA(18) = R(or RERUN)
2	2 - 7		&RERUN
	9 etc.		NAMELIST NAMES as described below, &END

HMAX: see CARD 4 of the section 5.2.

HFMAX: "

HPRINT: "

HDPZE "

CARD	COLUMNS	FORMAT	SYMBOL

HDPMX: see CARD 4 of the section 5.2.

HFDPZE: "

HFDPMX: "

NSPQSM: "

QRERUN: "

5.5.2 The Rerun for Performing a Small Effect Calculation

The SMEC option allows the calculation of small effects in certain geometr regions specified by LQS(N), N=1, LQSM (card 4). If in the course of the r dom walk process a neutron enters such a specified region, its coordinates all other characteristic parameters (energy, weight, direction, etc.) are stored on Data Set 11 and the history is terminated. The results of this f sampling procedure represent the "Basic Case". Its physical meaning would l the regions LQS(N) are black.

In a subsequent small effect calculation (RWS-SMEC-step), histories whose parameters are stored on Data Set 11 are read consecutively from it - if required splitted - and in the case of an eigenvalue calculation, ITER opt iterated. Finally they are combined with the "Basic Case" stored on the Re file on Data Set 10.

There are two possibilities for Small Effect calculations:

A) A SMEC calculation which is performed for the isotope composition defin originally in the NDP program for the regions LQS(N), N=1, LQSM.

CARD	COLUMNS	FORMAT	SYMBOL
1	1 - 60	15A4	COMCA(N),N=1,15
	COMCA(N),N=1,15 job identification corresponding to the basic case		
	61	1A1	COMCA(16) = R (or RWS)
	67	1A1	COMCA(17) = S (or SMEC)
2	2 - 7	&RERUN	
			NAMELIST NAMES (See previous section)
		&END	

B) Small Effect Calculations which are performed for other isotope compositions of LQS(N), N = 1, LQSM than used in A). In this case the complete input of NDP and RWS has to be repeated with the required changes of the isotope mixtures of LQS(N) and the following changes of COMCA(17) of the job identification card.

Input Parameters for the 1st Link Job (NDP)

1	1 - 60	15A4	COMCA(N),N=1,15
	COMCA(N), N = 1,15 job identification corresponding to the basic case		
	61	1A1	COMCA(16) = N
	67	1A1	COMCA(17) = N
2 to 20	as in the basic case with the exception of the changes necessary to redefine the regions LQS(N), N = 1, LQSM.		

Input Parameters for the 2nd Link Job (RWS)

1	1 - 60	15A4	COMCA(N),N=1,15
	COMCA(N)=1,15 job identification corresponding to the basic case.		

CARD	COLUMNS	FORMAT	SYMBOL
	61	1A1	COMCA(16) = R
	67	1A1	COMCA(17) = N
2 to 4	as in the basic case.		

6. PLOTGEOM: A PROGRAM FOR DISPLAY OF GEOMETRY BY MEANS OF A CALCOMP PLOTTER

6.1 Introduction

PLOTGEOM is a program for checking both the geometry subprogram and the geometry input data of Monte Carlo particle transport codes. It applies the geometry subprogram in a similar way to a random walk program. From the points of intersection between the geometrical structure and a mesh of lines of flight, PLOTGEOM generates a picture, representing a cross-section of the geometry.

The version described here has been connected with the O5R-Geometry Program (1).

The plot routines are completely described in (2). Other geometry and plot programs can easily be incorporated.

6.2 Method

The user specifies a two-dimensional cross-section of the geometry by giving its orientation with respect to the geometry coordinate axes and the desired coordinates of the corners of the picture[1].

The program generates a horizontal grid of lines (parallel to the x-axis of the picture), covering the area of the desired picture (Notation: L_i). The constant distance ϵ between the lines L_i and L_{i+1} is 0.07 cm in the picture. The points of intersection with the medium boundaries are re-

---

1) Note that the x-y coordinate system of the "picture" is usually different from the one to which the geometry description refers.

corded. Using for the start point the notation $P_{i,o}$ and for the crossing points $P_{i,j}$ one can write the distance between the start and crossing point $P_{i,j}$ as

$$d_{i,j} = P_{i,j} - P_{i,o}$$

After having scanned line L_{i+1} the following can be concluded. If

$$\left| d_{i,j} - d_{i+1,k} \right| \leqslant \frac{1}{2} \varepsilon$$

then the linepiece $\overline{P_{i,j}\ P_{i+1,k}}$ is called a segment. If more than one $P_{i+1,k}$ satisfies the quoted condition then only the nearest one to $P_{i,j}$ is taken.

Now we define a body as being one segment or a string of segments, so that the endpoint of one segment is the begin point of the next segment.

If a body with a last point $P_{i,j}$ already exists, the segment $\overline{P_{i,j}\ P_{i+1,k}}$ is connected to this body and the last point of that body becomes $P_{i+1,k}$.

If there is no body having $P_{i,j}$ as last point, the segment $\overline{P_{i,j}\ P_{i+1,k}}$ is the first one of a new body and the program looks for a "head" to be connected to $P_{i,j}$. This "head" has to be in the neighbourhood of $P_{i,j}$ between L_i and L_{i-1} and is found by the subroutine HEADTL. The same principle as that for finding the segments is applied by HEADTL. This subroutine uses however a refined and variable grid.

Calling the lines ℓ_m and the points $p_{m,n}$ the distance δ between ℓ_m and L_i may be between $2^{-6}\varepsilon$ and $(1-2^{-6})\varepsilon$ depending on the result of

ℓ_{m-1}. The first δ used is $\frac{1}{2}\varepsilon$. The start point is determined by:

$$\left| P_{m,o} - P_{i,j} \right| = \frac{1}{2}\sqrt{2}\,\delta .$$

The length of ℓ_m is $2\,\delta$.

If there is a body with a last point $P_{i,j}$ and if on examining L_{i+1} no segment $\overline{P_{i,j}\,P_{i+1,k}}$ is found, then this body should be given a "tail". This tail is determined by the subroutine HEADTL in the same way as a head, but now between L_i and L_{i+1}.

The "worms" (head, body, tail) thus created are stored on disk.

If the horizontal scanning has been finished the same procedure is repeated in the vertical direction (parallel to the y-axis of the picture).

Finally the worms are concatenated as far as possible: head to tail, head to head, tail to tail. The strings of worms formed in this way are plotted.

Remarks:

1. The grid distance of 0.07 cm is based on a picture dimension of at most 70 cm, so that no more than 1001 parallel lines L_i are possible.

2. A maximum of 30 crossing points are accepted in one line. If the cross section has more, two pictures must be made.

3. A closed surface, where the equivalent dimensions in the picture are less than 0.07 cm, may not be detectable. Distances between surfaces

of less than 0.07 cm in the picture may cause the contours to run into each other.

4. The quoted dimensions can easily be changed in the program.

6.3 Input of the Program PLOTGEOM

The data deck consists of cards with a control function, so-called directive cards, and cards with data. Each action (thus also the reading of data cards) is preceded by a directive card. The first card expected by the program is therefore a directive card. Having finished the execution of a directive, the program expects a new directive till it has executed the directive ØSTØP. The format of a directive card is 20A4. In column 1 must be placed the Ø sign. The actual directive takes the column 2 till 5 inclusive. The rest of the card is free for comment. Cards without Ø are automatically ignored.

Directives + supplementary data

ØTITLE - The program expects as next card a title card in the format 20A4.

ØDATA - The program expects the data cards for the geometry description.

N.B. For the O5R-geometry the 1st card contains the in- and output data set reference number in the 2I6 format.

ØSTOP - The program is terminated.

ØCALComp - The logical variable CALC is set equal .TRUE. . The initial situation is CALC=.FALSE. If CALC=.TRUE. the data to be plotted will be written on the calcomp tape.

ØNOCAlcomp - CALC is set .FALSE. .

ØHISTory - HIST is set .TRUE. . The initial situation is HIST=.FALSE. If HIST=.TRUE. the coordinates in the startpoint of the flight and in the points of intersection of the flight path with the geometrical structure are printed.

ØNØHIstory - HIST is set .FALSE. .

ØDESPrint - DESP is set .TRUE. . The initial situation is DESP=.FALSE. If DESP=.TRUE. the scaled data to be plotted will also be printed.

ØNØDEprint - DESP is set .FALSE. .

ØMEDIa - MEDI is set .TRUE. . The initial situation is MEDI=.FALSE. If MEDI=.TRUE. the program expects in the following cards the coordinates of points in the geometry. For these points the medium numbers will be plotted in the picture. The projection of such a point on the picture determines the lower left position of the plotted symbol(s). It is clear that this directive only has meaning if it follows ØPAUT. The expected cards are:

A: Format ($\overset{a}{I6}$,$\overset{b}{E12.5}$)

a - The number of points
b - The height of the numbers, to be written, in CM.

B: Format ($\overset{a,b,c}{3E12.5}$)

a - x-coordinate
b - y- "
c - z- "

For each point there has to be one card.

ØNØMEdia - MEDI is set .FALSE. .

ØØRIHin - ØRIG is set .TRUE. . The initial situation is ORIG=.FALSE. If ØRIG=.TRUE. the program expects in the following card two numbers X and Y in the Format (2E12.5). These numbers are used in the plot of the scale numbers along the X- and Y-axis of the design as the origin.

ØNØØRigin - ØRIG is set .FALSE. .

$PLINe - The program expects in the next card the coordinates X1, Y1, Z1 of point P1 and the coordinates X2, Y2, Z2 of point P2. Format (6E12.5). Next, P1 and P2 are connected and all points of intersection will be printed.

$PPNT - The program expects in the next card the coordinates X1, Y1, Z1 of point P1. Format (3E12.5). Next, the material in P1 is printed.

$PAUTomatic - The program expects the following cards:

Card A: Format (6E10.5)

a. XO the coordinates of the point in the geo-
b. YO metry that forms the lower left corner of
c. ZO the picture.

d. X1 The coordinates of the point in the geo-
e. Y1 metry that forms the upper right corner
f. Z1 of the picture.

Card B: Format (6E10.5)

a. XD These parameters are proportional to the
b. YD direction cosines of the direction of the
c. ZD Y-axis of the design.

d. XA These parameters are proportional to the
e. YA direction of the direction of the X-axis
f. ZA of the design.

Card C: Format (3E10.5)

a. XCM The width of the picture
b. YCM The height of the picture
c. SCFCT The scale factor from real measures to picture. Remark: a,b or c should be indicated.

Next, the program starts the scanning of the defined plane in order to create the lines of intersection of plane and geometrical structure. If CALC has been set. TRUE. these pieces of the picture are temporarily stored on disk and afterwards loaded on the Calcomp tape.

Remarks:

1. If the upper side or the right side of the picture coincides with an outer boundary of the geometry then it

may happen that, due to rounding errors, the last line of flight is outside the geometry. The O5R program will then stop. In such a case one should keep the picture a bit in the geometry.

2. The use of direct access input/output statements in subroutine PLØTG1 makes the definition of two data files on scratch disks necessary. The plot subroutines used in this version store the data to be plotted on data set 16.

   The DD cards used at the Euratom installation are:

```
//GØ.FT01FOO1  DD DCB=(RECFM=F,LRECL=7200),
//         SPACE=(CYL,100),UNIT=SYSSQ,
//         DISP=(NEW,DELETE,DELETE),
//         VØL=SER=(EURSY2)
//GØ.FT02FOO1  DD DCB=(RECFM=F,LRECL=7200),
//         SPACE=(CYL,100),UNIT=SYSSQ,
//         DISP=(NEW,DELETE,DELETE),
//         VOL=SER=(EURSY3)
//GØ.FT16FOO1  DD UNIT=TP9,LABEL=(,,,ØUT),
//         DSN=dsname,VØLUME=(PRIVATE,SER=EUnnnn),
//         DCB=(,DEN=2,TRTCH=C,RECFM=VS,
//         LRECL=484,BLKSIZE=488)
```

6.4 Short Description of the Program

The program deck to be used consists of four groups of subroutines.

1. The PLOTGEOM Programs:

Name	Subroutines used
MAIN	PLOTGM
PLOTGM	PLINPT, PLOTG1, PLSCAN, PLOTG5, PLOTG4
PLINPT	HEAD, HEADR, PLINE, INPUT, PLPNT, PLFIN, PLOTDS, PLOTG6

PLOTDS	
PLSCAN	PLOTG2, CROSS, HEADTL, PLOTG3
HEADTL	CROSS
PLOTG1	FINIM, SYMBL4, AXPL, HEAD, LINE,
(PLOTG2)	PLMED, NUMBER, FINTRA
(PLOTG3)	
(PLOTG4)	
(PLOTG5)	
(PLOTG6)	
(PLFIN)	
CRØSS	START, PATH
PLINE	CRØSS
PLPNT	PLMED
AXPL	NUMBER, PLØT
HEAD	
(HEADR)	
BLOCK DATA	

2. The connecting programs between the PLOTGEOM and the Geometry Programs:

Name	Subroutines used
PLMED	START
INPUT	JOMIN
START	LOOKZ
PATH	GEOM

3. The plot programs (see (2))(in Ispra in the System Library).

FINIM

FINTRA

LINE

NUMBER

SYMBL4

PLOT

4. The Geometry Programs. See (1).

6.4.1 Explanation regarding some important subroutines

The dimension of the vector X in COMMON (used in the O5R Geometry for data storing) is defined in the MAIN program. The MAIN program calls PLOTGM which executes the following steps:

1. Calls PLINPT which reads and prepares the input.
2. Calls PLOTG1 to prepare the plotting.
3. Prepares the parameters for the horizontal scanning.
4. Calls PLSCAN which scans the cross section in the horizontal direction of the picture. The "worms" are stored on disk.
5. Prepares the parameters for the vertical scanning.
6. The same as in 4., now in the vertical direction.
7. Calls PLOTG5 to concatenate the "worms" from disk and to plot the strings thus formed.
8. Calls PLOTG4 to position the coordinates for the next design.
9. Return to 1.

Subroutine PLINPT reads and interprets the directives. It reads, prints and stores the connected data. With the exception of PAUT all directives are executed by PLINPT calling the appropriate subroutines. In the case of PAUT the control returns to the calling program PLØTGM.

Subroutine PLOTG1 with the other entries PLOTG2, PLOTG3, PLOTG4, PLOTG5, PLOTG6 and PLFIN takes care of the plotting. It stores, retrieves, scales and plots the desired data. All plot routines are called by means of this subroutine.

Subroutine PLMED (X,Y,Z,M)

Determines in the point (X,Y,Z) the material number M.

Subroutine INPUT

Calls for the input subroutines of the geometry program after having determined the necessary arguments.

Subroutine START (XB,YB,ZB)

Sets the parameters in the geometry program for a flight vector starting in the point (XB,YB,ZB).

Subroutine PATH

Computes the distance from the actual position along the line of flight to the next point of intersection.

6.5 Description of COMMON and Variables

/PLGE1/ shared by PLØTGM, CRØSS

XC, YC, ZC — The direction cosines of the line of flight.

XPDEL — The distance between two sequential points of intersection.

XREST — The remaining part of the line of flight.

XE, YE, ZE — The coordinates of the endpoint of the line of flight.

IX — Event index = 0 = intersection.
1 = end of flight (collision).

/BLPATH/ Shared by CRØSS, PATH

XP, YP, ZP — Start point of the line of flight.

/PLGE2/ Shared by PLSCAN, HEADTL, PLOTGM

XP1, YP1, ZP1 — The lower left point of the picture in the geometry (point P1).

A — The distance from P1 to the lower right point.

EPS — The distance between two normal parallel lines of the grid.

DXD, DYD, DZD — The increments of the start coordinates for the next parallel line of the grid.

XA, YA, ZA — The direction cosines of the actual lines of the grid.

IENT — A counter for the number of CALL's of CRØSS.

IMAX — The number of grid lines.

XD, YD, ZD — The direction cosines of the normal of the grid.

/PLGSPE/ Shared by BLØCK DATA, CRØSS, PLINPT, PLOTGM

SPECIF(20) Images of specifications (directives).

SQ(20) Logical variables defining the state of the corresponding specification in SPECIF.

/PLGE3/ Shared by PLSCAN, HEADTL, CRØSS

JC — The number of intersections made in subroutine CRØSS.

C(30) The distances between the start point of the neutron along the line of flight and the points of intersection.

/PLDATA/ Shared by PLSCAN, PLØTG1

LH(30)	Nb. of head points
LT(30)	Nb. of tail points
PDX(1005,30)	x-coordinates of body points
PDY(1005)	y- " " " "
NXI(30)	Index first point of body
LXI(30)	" last " " "
HPDX(10,30)	x-coordinates of the heads
HPDY(10,30)	y- " " " "
TPDX(10,30)	x- " " " tails
TPDY(10,30)	y- " " " "

/PLGE4/ Shared by PLOTGM, PLOTDS, PLOTG1

XO, YO, ZO	Geometry coordinates defining the lower left corner of the picture.
XHR, YHR, ZHR	The direction cosines of the y-axis of the picture.
XWR, YWR, ZWR	The direction cosines of the x-axis of the picture.
WRECTA	The dimension of the cross section along the x-axis.
HRECTA	The dimension of the cross section along the y-axis.
XCM	The width of the picture = WRECTA*SCFCT (CM).
YCM	The height of the picture = HRECTA*SCFCT (CM).
SCFCT	The scaling factor.
DELD	Mesh in geometry.

SCANX	Logical constant. True = Scanning in horizontal mode. False = Scanning in vertical mode.

/PLGE5/ Shared by PLINPT, PLØTG1

NBMED	The number of points of the geometry of which the medium number should be plotted.
SYMBH	The height of the number to be plotted in CM.
CØMED(3)	The coordinates of the points.
XØR YØR	Values of the graduation in the origin of the design.

6.6 References

(1) D.C. Irving, R.M. Freestone,Jr., F.B.K. Kam - 05R, A General Purpose Monte Carlo Neutron Transport Code, Oak Ridge 1965, ORNL-3622.

(2) P. Moinil, J. Pire - Programmation Relative au CALCOMP, Ispra 1965, EUR 2280.f.

6.7 Sample Problem

The Sample Problem consists of two concentric cones.

6.7.1 Input Data for the Sample Problem

```
$DATA
     5       6
     2      MALE
X-ZONE BOUN   -5.000  ,   5.000                                          A
Y-ZONE BOUN   -5.000  ,   5.000                                          B
Z-ZONE BOUN   -5.000  ,   5.000                                          C
ZONE          1     1     1                                            D
BLOCK BOUNX   -5.000  ,   5.000                                          E
BLOCK BOUNY   -5.000  ,   5.000                                          F
BLOCK BOUNZ   -5.000  ,   5.000                                          G
BLOCK         1     1     1                                            H
MEDIA              1,    2,    3                                       J
SURFACES           1,    2                                             K
SECTOR -1  0                                                           L
SECTOR  1 -1                                                           1M
SECTOR  0  1                                                           2M
                                                                       3M
     2    QUADRATIC SURFACES (CONES)
  1.0       XSQ     1.        YSQ      -0.25     ZSQ   $
  1.0       XSQ     1.        YSQ      -1.       ZSQ   $
$CALCOMP
$TITLE
FIG.2 - 2 ELLIPSES
$PAUT
   5.0        -5.0       -4.0        -5.0        5.0         0.0          ELLIPSES
  -1.0         0.0        0.0         0.0        0.9285      0.436        ELL.
                          1.
$TITLE
FIG.5 - 2 HYPERBOLAS
$PAUT
   1.0        -5.0       -5.0        -1.0        5.0         3.0          HYPERB.
  -0.242       0.0        6.965       0.0        1.0         0.0          HYPERB.
                          1.
$STOP
```

6.7.2 Output of Sample Problem

```
$DATA

     2      MALE
X-ZONE BOUN -0.50000D 01,   0.50000D 01
Y-ZONE BOUN -0.50000D 01,   0.50000D 01
Z-ZONE BOUN -0.50000D 01,   0.50000D 01

ZONE        1     1     1
BLOCK BOUNX -0.50000D 01,   0.50000D 01
BLOCK BOUNY -0.50000D 01,   0.50000D 01
BLOCK BOUNZ -0.50000D 01,   0.50000D 01

BLOCK       1     1     1
MEDIA             1,     2,     3
SURFACES          1,     2
SECTOR -1   0
SECTOR  1  -1
SECTOR  0   1

    2  QUADRATIC SURFACES (CONES)
  0.10000D 01XSQ       0.10000D 01YSQ      -0.25000D 00ZSQ   $
  0.10000D 01XSQ       0.10000D 01YSQ      -0.10000D 01ZSQ   $

$CALCOMP

$TITLE


PLOTGEOM**FIG.2 - 2 ELLIPSES

$PAUT

PARAMETERS USED

XO=    0.50000E 01
YO=   -0.50000E 01
ZO=   -0.40000E 01

X1=   -0.50000E 01
Y1=    0.50000E 01
Z1=    0.0

XD=   -0.10000E 01
YD=    0.0
ZD=    0.0

XA=    0.0
YA=    0.92848E 00
ZA=    0.37139E 00

XCM=    0.10770E 02
YCM=    0.10000E 02
SCFCT=    0.10000E 01

SUBROUTINE CROSS HAS BEEN ENTERED  203TIMES

SUBROUTINE CROSS HAS BEEN ENTERED  413TIMES


     8 WORMS HAVE BEEN STORED ON DISK AND ARE NOW PLOTTED
```

Output of Sample Problem (cont.)

```
$TITLE

PLOTGEOM**FIG.5 - 2 HYPERBOLAS

$PAUT
PARAMETERS USED

XO=    0.10000E 01
YO=   -0.50000E 01
ZO=   -0.50000E 01

X1=   -0.10000E 01
Y1=    0.50000E 01
Z1=    0.30000E 01

XD=   -0.24325E 00
YD=    0.0
ZD=    0.96996E 00

XA=    0.58489E-03
YA=    0.10000E 01
ZA=    0.14687E-03

XCM=    0.10000E 02
YCM=    0.82462E 01
SCFCT=    0.10000E 01
SUBROUTINE CROSS HAS BEEN ENTERED  135TIMES
SUBROUTINE CROSS HAS BEEN ENTERED  389TIMES

     12 WORMS HAVE BEEN STORED ON DISK AND ARE NOW PLOTTED

$STOP
```

6.7.3 Calcomp output of the Sample Problem

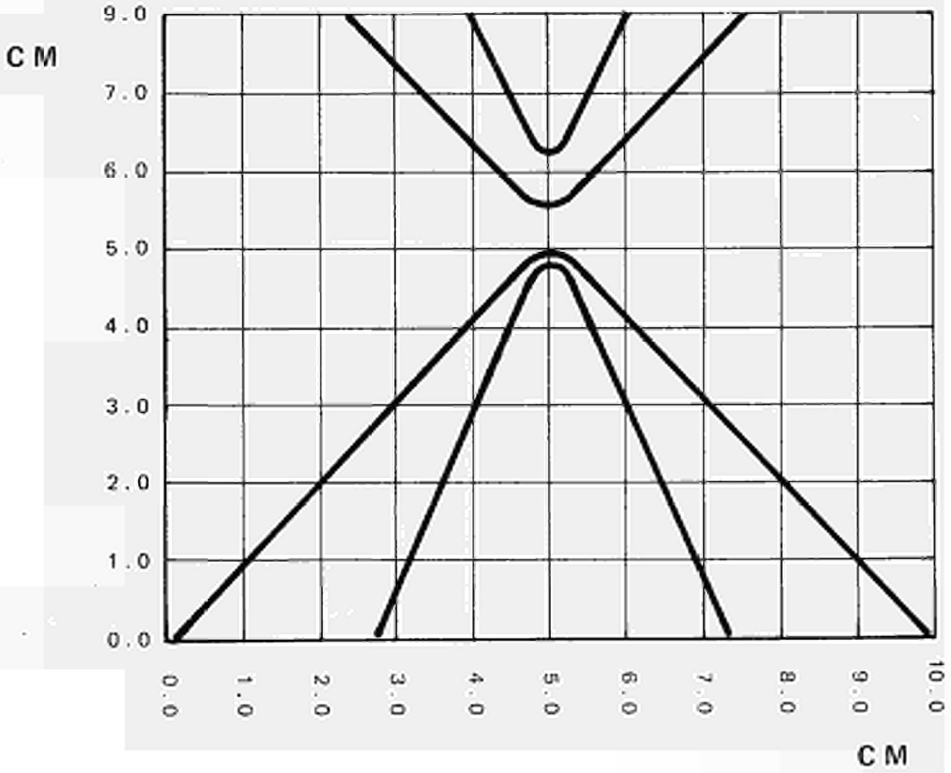


FIG. 5 – 2 HYPERBOLAS

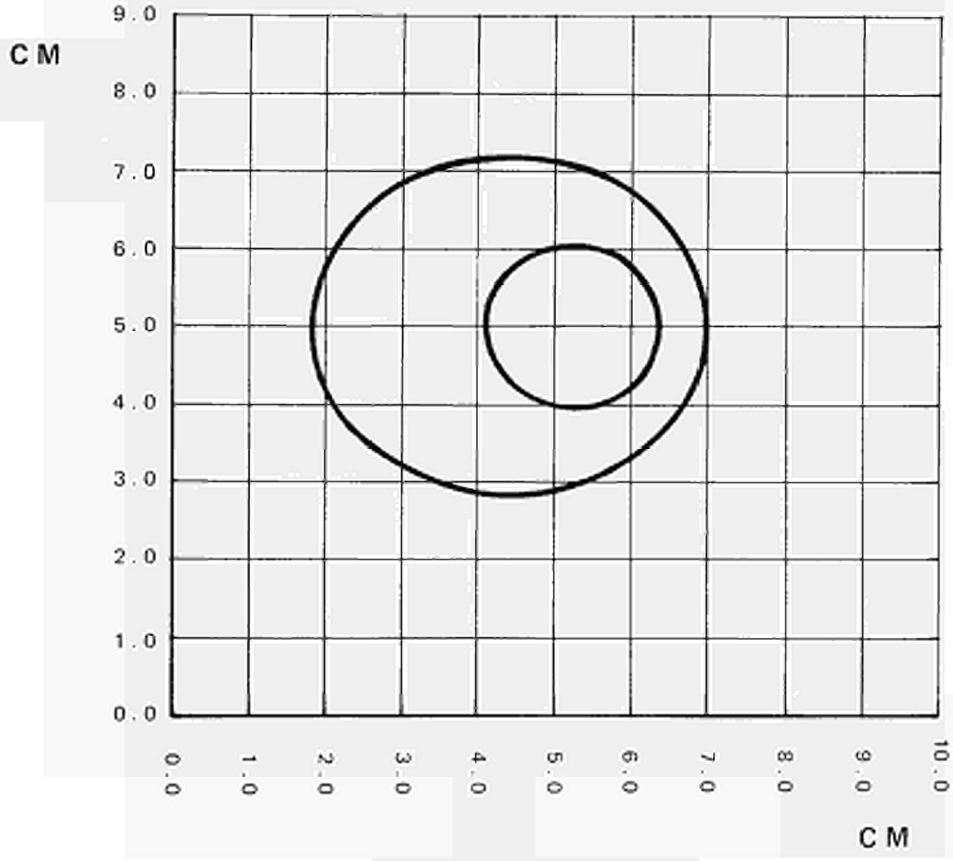
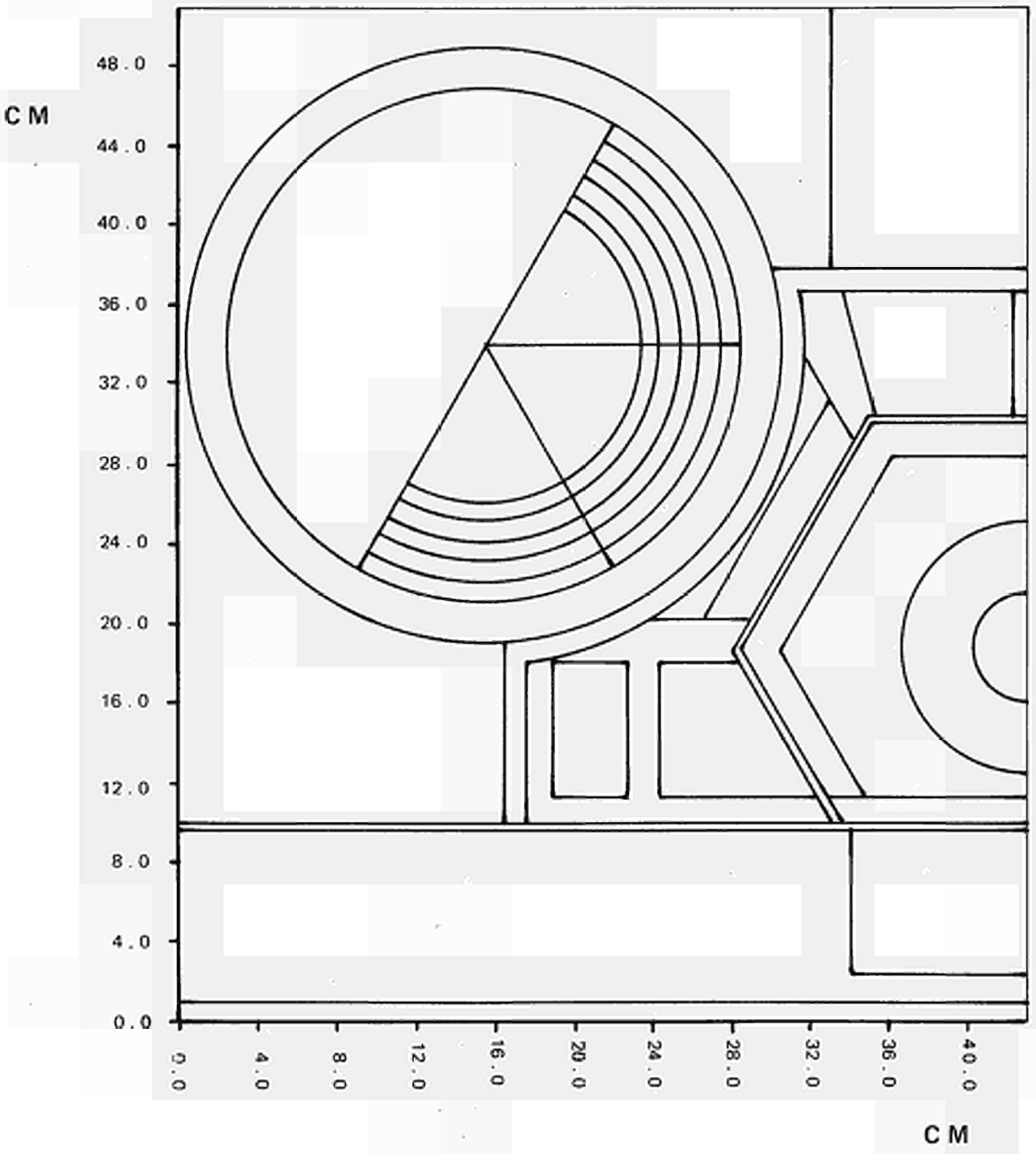


Fig. 2 – 2 ELLIPSES

6.7.4 Practical example of Calcomp output



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Appendix A - Geometry Program

1. The geometry subroutines GINOUT, GSTRT, GPATH and GEOPJ

General

The geometry module is interfaced through the following four subroutines:

GINPUT (NIN,NOUT) - reads prints and develops the parameters describing the geometrical structure and the starting points.

GSTRT (X,Y,Z,MED,PK1) - determines the initial space parameters of a new neutron.

GPATH (X,Y,Z,U,V,W,MED,PK1,PTD,FRP,SGT,ID1) - determines the space parameters of the next collision point if the neutron flight lays in the actual medium, or of the medium boundary crossing point if encountered before the end-of-flight.

GEOPJ (U,V,W,T) - determines the cosine of the angle between the line of flight and the surface normal in the point where the medium boundary has been crossed.

The data transfer from GINPUT to GSTRT and GPATH takes place via blank and labeled common, therefore GINPUT and its subroutines may be placed in another overlay segment.

The meaning of the arguments is:

NIN - The Fortran reference number of the input data set of the Geometry Data.

NOUT - The Fortran reference number of the output data set of the Geometry Data.

X
Y
Z — Space coordinates, defining the position of the neutron.
DOUBLE PRECISION.

MED — The medium index.

PK1 — A DOUBLE PRECISION word containing supplementary space parameters (only of internal interest).

U
V
W — The components of the unit direction vector.
DOUBLE PRECISION.

PTD — The covered distance in cm between the event on entry and the event on return.

FRP — The number of mean free paths for the next flight.

SGT — The total cross-section of the actual medium.

ID1 — The event index
2 = A new neutron has been started (1st flight).
1 = The last event has been a collision.
0 = The last event has been a medium crossing.
-1 = The neutron has entered leakage.

T — The cosine of the angle between (U,V,W) and the normal to the surface in the last crossing point.
T is always positive.

The input of GPATH is: X,Y,Z,U,V,W,MED,PK1,FRP,SGT and ID1.

The output of GPATH is: X,Y,Z,MED,PK1,PTD,FRP and ID1.

Not modified are: U,V,W and SGT.

GEOPJ should be called immediately after the crossing of a medium boundary.

The input of GEOPJ is U,V,W.

The output of GEOPJ is T.

Not modified are: U,V,W.

Remarks

The subroutine GINPUT calls the subroutine JOMIN of the O5R, which reads, develops and prints all geometry data. The cards containing the starting point information are read, developed and printed by GINPUT, using the appropriate subroutines of O5R and its retrieval techniques. This information has been transfered to GSTRT by means of the vector DV in COMMON and the labeled common /GSTART/.

The subroutine GPATH prepares the arguments for the O5R routine GEOM, calls for GEOM and prepares the results again for the interface.

The subroutine GEOPJ calls the subroutine NORML, which determines the surface normal in the actual crossing point.

2. Modifications in the General O5R Geometry

I. JOM11

In the actual O5R geometry taken from the MORSE deck each block may contain 31 surfaces instead of 18 as has been written in the MORSE report. The input routine JOM11 to read the sector cards was nevertheless only prepared to read 18 sectors. This has been corrected now and the new version is on disk.

The input description of this card (= card M, page 51 of the ORNL-3622 report) becomes:

Card M: Format $(A6^{a},22I3/6X,9I3^{b})^{b}$

II. JOM14

The parameters NZ, NXBL, NYBL, NZBL, NBOUND and SGNF are unpacked from BLZON by the subroutine JOM14 and packed into BLZON by JOM15.

In the actual version BLZON is assumed to have single precision and this version has therefore the following limits:

63 SURFACES in the whole geometry
127 ZONES in the Whole geometry
62 BLOCKS for each AXIS in a ZONE.

These limits are only of importance if MARK = 1 or -1, that means if a neutron STARTS or RESTARTS its flight from a MEDIUM that is defined by ZONE, BLOCK and/or SURFACE being above the mentioned limits.

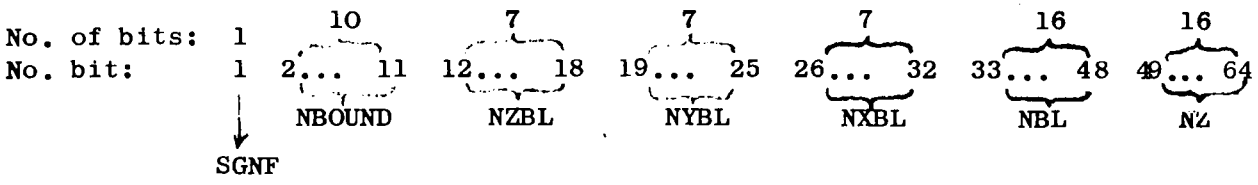
In TIMOC it may happen to:

a. Primary neutrons
b. Secondary neutrons
c. Neutrons stored on tape when entering the SMEC specified media.

To overcome all difficulties a new and faster version has been made that packs into the double word BLZON and that has the following limits:

1023 SURFACES
32767 ZONES and 32767 BLOCKS in each ZONE
126 BLOCKS for each AXIS in a ZONE.

The packed double word has the following representation:



Appendix B - Random Number Package

- The random number package of TIMOC 71 is an extension of the O5R package.

- The O5R package contains a Multiplicative Random Number Generator

$$t_{k+1} \equiv \lambda_2 \, t_k \pmod{P}$$

where $\lambda_2 = 5^{15} - 7 * 16^8$

$P = 2^{47}$

$t_o = 5^{15}$ (O5R) [Remark $t_o = 2 * (5^{15} - 7 * 16^8)$ in the MORSE code]

- The extension has been the generation of the initial history random number, that means the t_o's for the O5R generator.

This new generator may be written as:

$$t_o^{i+1} \equiv \lambda_i \, t_o^i \pmod{P}$$

From (1) is found that a good MRNG is achieved

if $\lambda_1 \equiv \pm 3 \pmod 8$ and λ_1 as great as possible.

Therefore we have taken $\lambda_1 = 3^{21} - 2 * 16^8$

$P = 2^{47}$

$t_o^o = 1$

---

(1) R.R. COVEYOU - Random Number Generation is too Important to be left to Change (National Meeting of Society for Industrial and Applied Mathematics, Washington, June 11-15, 1967).

Both generators have the period 2^{45} and the Random Numbers are in (0,1).

- The program described in (2) has been used to test the combination and it has been found that the distribution is sufficiently uniform and free of correlations. The tests are listed in Table 1.

TABLE 1

Type of generated Random Number	Number of RNB	Type of Test
Original FLTRNF generator t_k, k = 1,2,... $t_o = 5^{15}$	3 x 10000 (k=1,2,...10000; k=10001,10002,...20000; k=20001,20002,...30000)	Uniformity test, 100 intervals
	3 x 10000	" " 10 "
	3 x 10000	" " 4 "
	3 x 50000	Pairs test on unif., 10 int.
	3 x 30000	Triples " " " 10 "
	3 x 100000	Max.,Min.,sum test M = 10
	3 x 100000	" " " M = 5
	3 x 100000	" " " M = 2
	32 sets of each 1024	Runs tests
The 1st RNB in each history t_1^i i = 1,2,3,...	The same	The same
The 1st 200 RNBN in each history t_k^i i = 1,2,3,... k = 1,2,3,...200	The same	The same
The 1st 200 RNBN in each 50th history t_k^i i = 1,51,101,... k = 1,2,3..200	The same	The same

(2) G. Fassone and S. Orthmann - A Test Program for Pseudo-Random Numbers with Uniform Distribution. EUR 3464.e.

Added and modified entries

CALL RNDIN2(R) Loads R into RANDOM
CALL RNDOT2(R) Loads RANDOM into R

CALL RNDIN(R) Loads R into RAND1
CALL RNDOUT(R) Loads RAND1 into R

R has to be in double precision and is written or read in the Z12 format. It occupies the last 6 bytes of RANDOM and RAND1.

The standard value of RAND1 = 1 ($\equiv t_o^o$)

RANDOM = 5^{15} ($\equiv t_o$)

The above named subroutines may serve to set initial values and to print the last RNB. If R = 0 the standard values are taken.

R = RNINI(0) causes the replacement of t_o^i by t_o^{i+1} and can be used before a new history is started. R and 0 are dummies.

The already existing function R = FLTRNF(0) replaces

$$t_k^i \text{ by } t_{k+1}^i$$

and stores the normalized RNB in R.

Appendix C - The Collision Subroutines INSC and ELSC

The collision subroutines INSC and ELSC

1. General

The collisions are handled by the subroutines:

INSC (NBAD,U,V,W,E,I) (inelastic scattering)
ELSC (NBAD,U,V,W,E,I,K) (elastic scattering).

These subroutines belong to the same module as the Random Walk Sampling programme RWS. The common data stores are in blank COMMON (the array DV equivalent with IDV and ENE) and in the labeled COMMON/NDRWS/.

The meaning of the argument is:

NBAD: The index of the 1st location of a subarray in the array DV that contains the nuclear data for handling collisions.
If NBAD = 0 the collision is isotropic in the c.m. system and no more information has been given in DV. NBAD must be determined in the calling programme.

U:
V:
W: } The components of the unit direction vector
D O U B L E P R E C I S I O N

E: The energy in Ev
I: The energy index — I = 0 means that the energy is less than the lowest energy limit. See also 2.1
K: The isotope index

The labeled COMMON/NDRWS/ contains:
(A is atomic weight, the index is K)

DUM(1) = dummy

A1(50) : $\frac{1}{1+A}$

A2(50) : $\frac{A}{1+A}$

A3(50) : $\frac{A-1}{A+1}$

A4(50) : $(\frac{A-1}{A+1})^2$

A5(50) : A^2-1

ATW(50) : A

The first locations of DV(=ENE) contain the energy boundaries. The description of the data in DV, used by these subroutines is given in the subroutine description.

The symbol ξ stands there for a random number between 0 and 1.
The O5R subroutine package for random numbers is applied.

2. Subroutine INSC (NBAD,U,V,W,E,I)

On entry the arguments should define the situation before the collision; on return the arguments define the situation after the collision.

LTT = IDV(NBAD) is an index defining the inelastic scattering description.
The scatterings are isotropic with a possible exception for LTT = 3.

2.1 LTT = 1: The model of excited levels is used

IDV(NBAD+1) contains 2 times the number NMAX of excited levels.
DV(NBAD+2N) is Δ E for the N-th energy level.
DV(NBAD+2N+1) is the cumulative probability for the N-th level.
(DV(NBAD+2·NMAX+1) = 1)

ΔE is DV(NBAD+2N) if $\xi < DV(NBAD+2N+1)$, N = 1 ... NMAX.
$E_{new} = E_{old} + \Delta E$. I is determined. If $E_{new} < 0$ and NMAX ≠ 1 the process is repeated. If $E_{new} < 0$ and NMAX = 1 or if E_{new} stays < 0 also after 100 repetitions: I = -1.

2.2 LTT = 2: The statistical (evaporation) model is used

IDV(NBAD+1) = 1

DV(NBAD+2) = T is the nuclear temperature

$E_{new} = -T \cdot Ln(\xi_1 \cdot \xi_2)$. If $E_{new} < E_{old}$ the process is repeated. I is determined.

2.3 LTT = 3: Energy transfer is described by a transfer matrix

IDV(NBAD+1) contains 3 times the number NMAX of the transfer probabilities.

IDV(NBAD-1+3N) is the new energy group.

DV(NBAD+3N) is the cumulative probability to scatter into the associated groups.

DV(NBAD+3N+1) is the average cosine of the angle of deflection in the Lab. system.

DV(NBAD+3NMAX) = 1

The new group is IDV(NBAD-1+3N) if $\xi <$ DU(NBAD+3N), N = 1,...NMAX.
E is taken at random in this group.

If DV(NBAD+3N+1) $\neq$ 0 the new direction is determined by the subroutine AVSCAT.

If IDV(NBAD-1+3N) is negative then it is assumed to be the negative value of the actual group and taken as a sign of down scattering in the actual group.

3. Subroutine ELSC (NBAD,U,V,W,E,I,K)

On entry the arguments should define the situation before the collision, on return they define the situation after the collision.

3.1 NBAD = 0: The collision is isotropic in the C system

The neutron speed $S = 1.383192 \times 10^6 \times \sqrt{E}$.
The incoming unit vector (U,V,W) is called $\vec{v}_1$.
The unit vector $\vec{v}_o$ is randomly generated.

The velocity vector after the collision is then given by:

$$\vec{V}_2 = \frac{S}{1+A}\,\vec{v}_1 + \frac{A}{1+A}\,S\,\vec{v}_o \qquad \text{and}$$

$$S_{new} = |\vec{V}_2| \qquad \text{and so}$$

$$E_{new} = \frac{S_{new}^2}{1.9132201 \times 10^{12}}$$; I is determined, and

the outgoing vector (U,V,W) is $\vec{V}_2/S_{new}$.

3.2 NBAD ≠ 0 and IDV(NBAD) = 1: The collision is anisotropic, defined by $\overline{\cos\gamma}$ (the average cosine of the angle of deflection in the L system)

$$DV(NBAD+1) = \overline{\cos\gamma}$$

From $\overline{\cos\gamma}$ and the incoming vector the subroutine AVSCAT determines the outgoing vector in such a way that the average of the inner product of these two vectors is equal to $\overline{\cos\gamma}$. If we call the actual inner product $\cos\gamma$ then

$$E_{new} = E_{old} \times \left\{ \frac{\cos\gamma + \sqrt{A^2 - 1 + \cos^2\gamma}}{(A+1)} \right\}^2$$

I is determined from E.

3.3 NBAD $\neq$ 0 and IDV(NBAD) $\neq$ 1. The collision is anisotropic in the C system, defined by a cosine boundary table of intervals with equal probability.

IDV(NBAD) = NMAX is the number of intervals.

DV(NBAD+N) = the lower boundary of the interval N. The upper boundary of the 1st interval has not been stored and is taken by the programme to be equal to 1.

$N = \xi \times NMAX+1$

From the N-th interval a discrete cos θ is selected assuming a uniform distribution over the interval.

If Υ is the corresponding angle of deflection in the L system then

$$\cos \Upsilon = \frac{1+A\cos\theta}{\sqrt{1+A^2+2A\cos\theta}}$$

$$E_{new} = E_{old} \times \frac{A^2+2A\cos\theta+1}{(A+1)^2}$$, I is determined.

The azimuthal angle Φ is defined by a uniform distribution in $(0,2\pi)$. Sin Φ and cos Φ are generated by AZIRN.

The vector (U,V,W) can be expressed in spherical coordinates as:

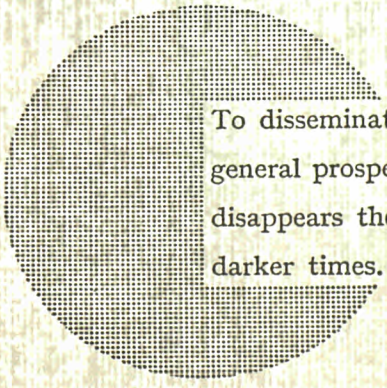
$$(\sin\theta_1 \cos\varphi_1 , \sin\theta_1 \sin\varphi_1 , \cos\theta_1).$$

Also the outgoing unit vector is:

$$U = \cos\varphi_1 \quad (\cos\theta_1 \cdot \sin\Upsilon \cdot \cos\Phi + \sin\theta_1 \cdot \cos\Upsilon) - \sin\varphi_1 \cdot \sin\Upsilon \cdot \sin\Phi$$

$$V = \sin\varphi_1 \quad (\quad \text{"} \quad) + \cos\varphi_1 \quad \text{"} \quad \text{"}$$

$$W = \cos\theta_1 \cdot \cos\Upsilon - \sin\theta_1 \cdot \sin\Upsilon \cdot \cos\Phi \ .$$



To disseminate knowledge is to disseminate prosperity — I mean general prosperity and not individual riches — and with prosperity disappears the greater part of the evil which is our heritage from darker times.

Alfred Nobel

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