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USER GUIDE TO LCS: THE LAHET CODE SYSTEM

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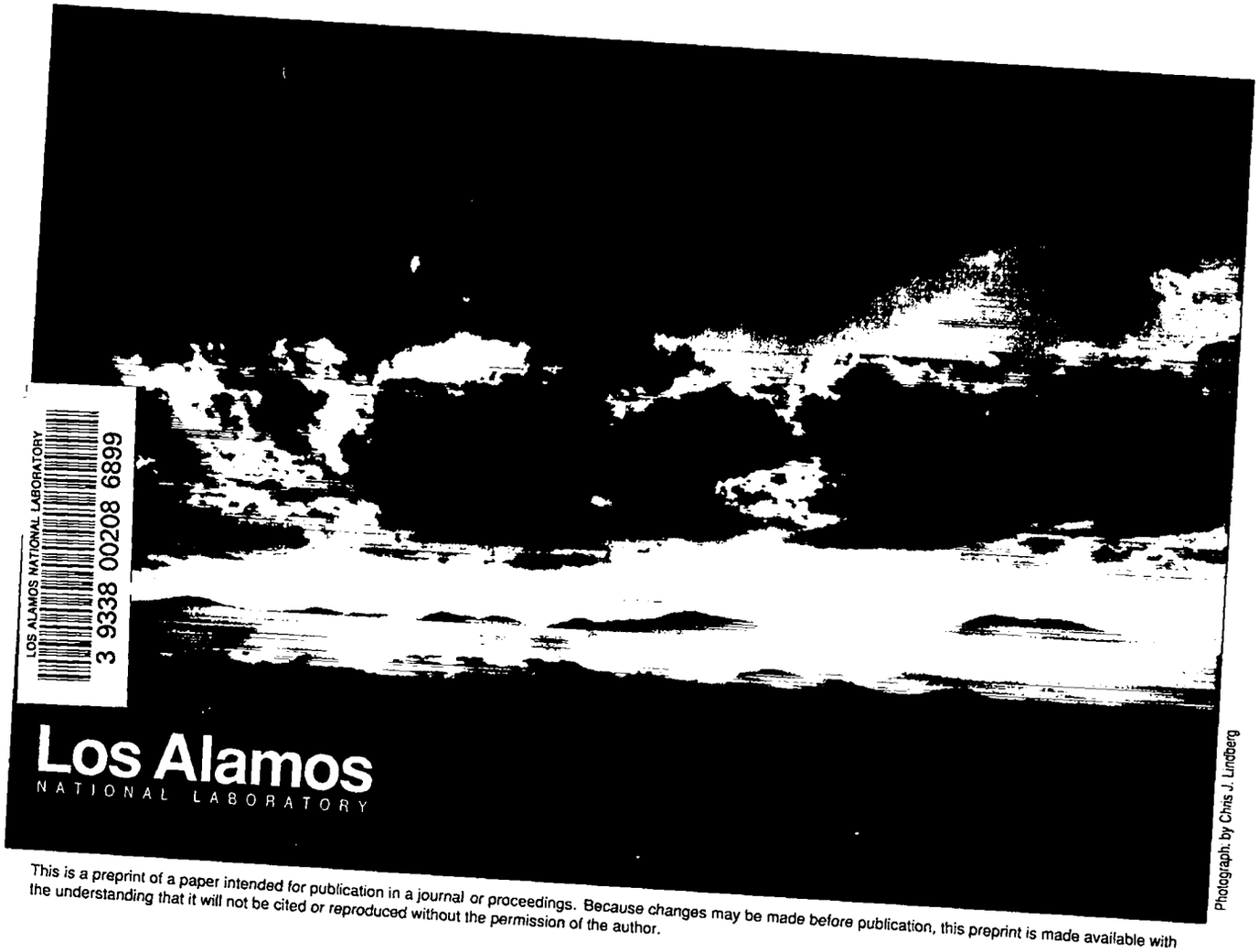

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User Guide to LCS: The LAHET Code System

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Chapter 1

INTRODUCTION

1.1 LCS: THE LAHET CODE SYSTEM

Over the past ten years, a major effort at Los Alamos National Laboratory has been the development of a code system based on the LANL version of the HETC Monte Carlo code for the transport of nucleons, pions, and muons, which was originally developed at Oak Ridge National Laboratory [1]. Due to the many new features added at LANL, the present release has been renamed LAHET, and the system of codes based on LAHET designated as the LAHET Code System (LCS).

In LAHET, the geometric transport capability is that of LANL's continuous energy neutron-photon Monte Carlo code MCNP[2]. LAHET includes as user options two models for fission induced by high energy interactions: the ORNL model by Alsmiller and others[3], and the Rutherford Appelton Laboratory model by Atchison[4]; the fission models are employed with the evaporation model of Dresner[6].

HETC utilizes the intranuclear cascade model of Bertini [5] to describe the physics of nuclear interactions. In LAHET, an alternative intranuclear cascade model has been adapted from the ISABEL code ([7],[8]), which allows hydrogen and helium ions and antiprotons [9] as projectiles. The ISABEL intranuclear cascade model is itself derived from the VEGAS intranuclear cascade code [11]. The Fermi breakup model [10] has replaced the evaporation model for the breakup of light nuclei. An optional multistage preequilibrium exciton model [12] has been implemented as an intermediate stage between the intranuclear cascade and the evaporation phase of a nuclear interaction. Alternative level density parameterizations have been added. A library of calculated neutron elastic scattering data has been provided.

The philosophy behind the HETC code has been to treat all interactions by protons, pions, and muons within HETC, but to treat neutron interactions only above a cutoff energy, typically 20 MeV at LANL. Any neutron appearing from a reaction with energy below the cutoff energy has its kinematic parameters recorded on a neutron file (NEUTP) for subsequent transport by a Monte Carlo code utilizing ENDF/B-based neutron cross section libraries. For LAHET, a version of MCNP (HMCNP) [13] which has been modified to accept NEUTP as an input source is used to complete the particle transport; recent development also allows proton and deuteron records to be passed to HMCNP for transport with the multigroup option of MCNP Version 3B [14].

Since the LCS is based on coupling LAHET to HMCNP via the neutron file, LAHET uses the MCNP geometry system. The user can most efficiently execute a computation by first preparing his HMCNP input file, using all the capabilities of that code to correct his geometric definitions; the HMCNP cell and surface records so generated may then be inserted into the LAHET input file with

few changes.

Calculational results from the HMCNP phase of the computation may be obtained directly from the standard MCNP tallies, although modified output edits appropriate to accelerator problems have been provided. Edited tallies of the initial LAHET run are obtained by subsequent processing of data recorded on the history file (HISTP) using the HTAPE code. The history file may contain a (nearly) complete description of the events occurring during the LAHET computation. One feature of HMCNP allows the writing of a history file called HISTX in a format similar to that of HISTP. The HISTX file may then be processed through the HTAPE code to obtain edits available only in HTAPE or in the same format as was obtained for the high-energy edits. At the present time, only selected surface-crossing events are recorded on HISTX.

The HMCNP phase of the computation may be executed as a coupled neutron-photon problem; however, to obtain a photon source from the high energy interactions computed by HETC, it is necessary to execute the PHT code. PHT accepts HISTP as an input file and produces a gamma file (GAMTP) containing a photon source for HMCNP in the same format as NEUTP. At the present time, the gamma source arises from two processes:

- The decay of neutral pions produced in the intranuclear cascade.
- The deexcitation of residual nuclei after all particle evaporation has ceased.

The two files, NEUTP and GAMTP, may be merged with the code MRGNTP to act as a source for HMCNP in a coupled neutron-photon problem which describes the transport of the entire gamma-ray source in the system. Alternatively, the two source files may be processed separately to analyze the effects of gammas arising from the high-energy interactions and the effects of gammas arising from neutron-induced reactions (below 20 MeV). The relationships of the various codes in the LCS and the files that carry information from one to another are shown in Figure 1.1.

LAHET may also be used to compute cross sections directly. With this option, the transport is turned off and the primary particle is assumed to interact directly with the specified material at the incident energy. The history file produced is then processed with the XSEX code to generate double-differential particle production cross sections.

1.2 A NOTE ON THE DOCUMENTATION

⇒ A new feature appearing in this edition of the documentation is that additions and changes since the last release (October 30, 1986) are flagged with a "⇒" or a "⇐" in the outer margin.

1.3 LIST-DIRECTED INPUT

Many of the input records for LAHET, HTAPE, XSEX, and PHT are input as "list-directed input". The rules for writing list-directed input as implemented for the LCS are as follows:

- The input data items in each record are free form with blanks, commas, or slashes as separators.
- A slash "/" as a separator designates the end of a record. When a slash terminates an input record before the input list is exhausted, the default values are assigned to the remaining input items. It is perhaps safest to *always* terminate a record with a slash.
- A null value (the default value will be used) is indicated by a comma (for the first item) or by two commas together.

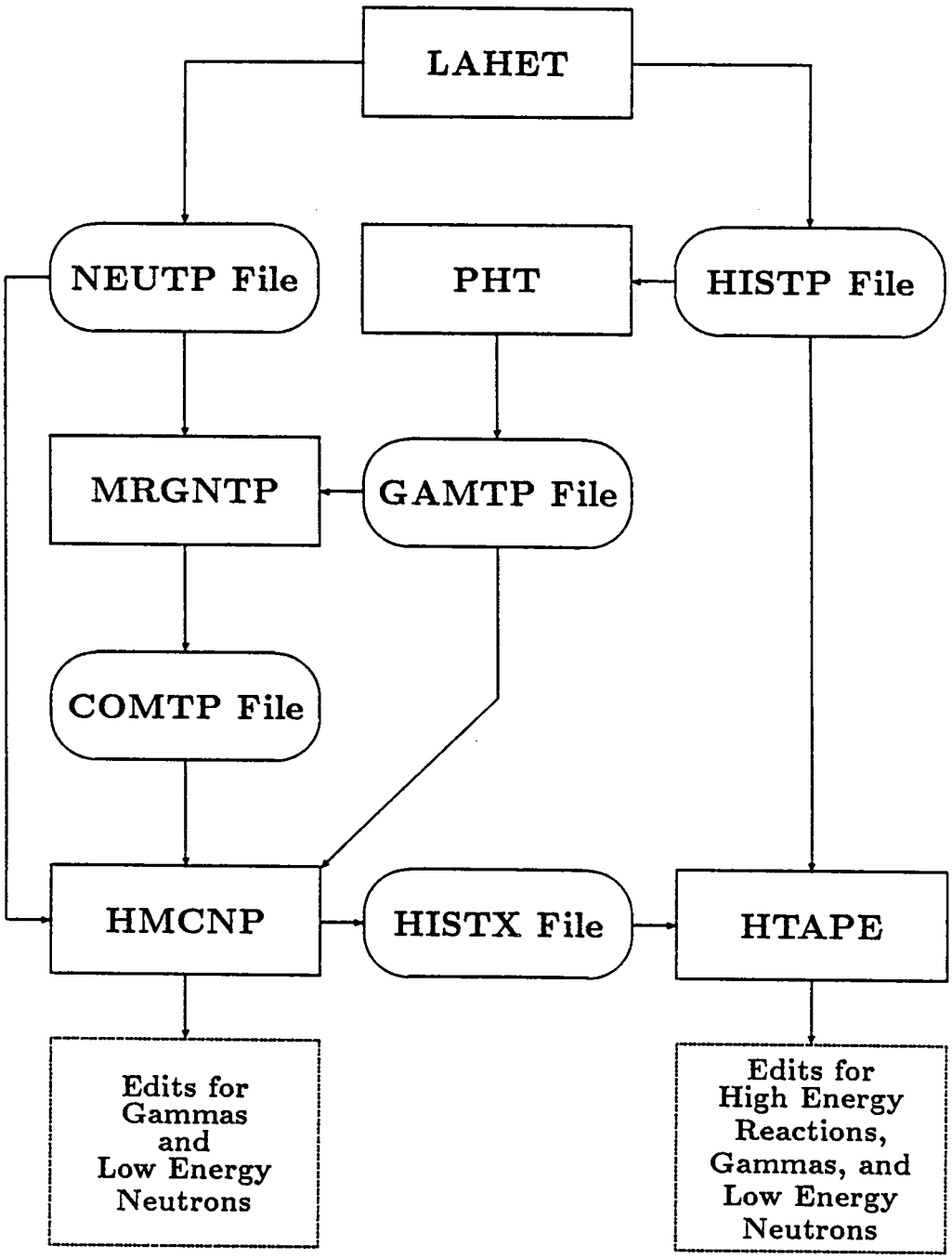

Figure 1.1: Code Linkage and Data Flow for the LAHET Code System

- Any remaining list items are treated as null when a slash appears.
- ⇒ Repeat counts may be used (3*2 is equivalent to 2,2,2 and 3*, is equivalent to ,,,).
- More than one record may appear on one line, provided the records are separated by slashes.
- A record may be continued to the next line.
- If multiple cases are to be processed in one execution (as with HTAPE), the title lines for the second and subsequent cases *must* begin with a "$" *if they contain a slash* "/".

1.4 FILE AVAILABILITY

For the current release, all files of the LCS are available from CFS node "/LCS" by executing

MASS GET /LCS/filename .

Chapter 2

THE LAHET CODE

2.1 LAHET INPUT FILE STRUCTURE (Version 2)

The bulk of the documentation available for LAHET has been provided for HETC by Oak Ridge National Laboratory [1]. The input file structure for LAHET as developed at LANL has been considerably changed from the HETC form described in [1] and from the more recent version of HETC in use at LANL. Some new parameters have been added and some old ones are no longer in use. A set of default values has been provided for most control parameters. Since LAHET uses the MCNP Version 2D geometry package [2], part of the input file has the MCNP file structure.

The full structure of the LAHET input file (conventionally named INH) is as follows.

- LAHET input records.
- Neutron elastic scattering data (if any).
- MCNP geometry input records.
- Source description records.

The neutron elastic scattering data, the MCNP geometry input, and the source description input are described below. The LAHET input records are as follows.

Record 1 First line of title.

Record 2 Second line of title.

Record 3 Format (Z12) with one item. A blank record must be supplied if only the default is desired. ⇐

RANDOM A 12-digit hexadecimal number for the starting random number; the default is 1123456789AB.

Record 4 List-directed with 14 data items.

MAXCAS The number of cascades in one batch; the default is 100 and must be > 0.

MAXBCH The number of batches to run; the default is 1 and must be > 0.

MXMAT The number of different media in the problem, exclusive of voids. The default is 1 and 0 < MXMAT ≤ 30 is required. *At least one material must be provided on records type 8 and 9, even though all cells may be void.* ⇐

NOELAS The total number of different nuclides for which neutron elastic scattering is to be considered and for which the user will supply data; the default is 0 and the maximum = 30. When using the neutron elastic scattering data file **/LCS/ELSTIN**, set NOELAS = 23 (see Section 2.2).

NLIMIT The maximum number of low energy neutrons to put on any one neutron file; the default is 400000 and zero takes the default. *Note: HMCNP allows only six files to be specified on the FILES record.* If the LAHET calculation will produce more than 2,000,000 low-energy neutrons to be transported with HMCNP, the parameter NLIMIT should be increased to prevent more than six neutron files from being written.

LHIST The maximum length of any one history file in decimal; the default is 10485760 ($= 50000000_8$) and zero takes the default. Insufficient disk space may prevent execution during daytime, with LAHET stuck in a "suspend" state waiting on disk space. In this case, a reduction of LHIST by a factor of two, or even four if necessary, will permit execution. Warning: since more files will be produced with a smaller length, the MXHIST limit (see below) may need to be large. Note the the LHIST parameter is entered as a decimal number, but appears on the output as an octal number.

NLBUF The output buffer length in decimal for neutron and history files. The default is 32768 ($= 100000_8$), zero takes the default, and the value is rounded up to a multiple of 10000_8internally.

JCASC Forces the calculation to start with history number JCASC in the sequence of random numbers defined by RANDOM; the default is 1 and JCASC ≤ 0 takes the default. The use of JCASC is primarily a debugging tool; it allows one to start a run with a particular history which may have occurred in a previous run which one may wish to examine. It is applicable only for NOSKIP ≥ 1.

IEXISA 0 ⇒ use Bertini model intranuclear cascade only (default);
1 ⇒ use Bertini model for nucleons and pions, with ISABEL model for other particle types;
2 ⇒ use ISABEL model for all incident particle types.
The ISABEL intranuclear cascade model requires a much greater execution time. In addition, incident energies should be less than 1 GeV, or 1 GeV per nucleon for composite particles (although it may execute at higher energies). See references [7], [8], and [9].

ICHOIC A composite of four integers in the form *ijkl* which define the options for the ISABEL intranuclear cascade model.

i = 0 ⇒ use partial Pauli blocking (default);
= +1 ⇒ use total Pauli blocking;
= -1 ⇒ no Pauli blocking (not recommended for anything).
The ISABEL code input variable IPAULI = $i + 1$.

j = 0 ⇒ no interaction between particles already excited above the Fermi sea (default);
> 0, the number of time steps to elapse between such "CAS-CAS" interactions.
The corresponding ISABEL code input variable is NTDEL, with default 3.

k = 0 ⇒ Myer's density prescription with 8 steps;
= 1 ⇒ original (isobar) density prescription with 8 steps;
= 2 ⇒ Krappe's folded-Yukawa prescription for radial density in 16 steps, with a local density approximation to the Thomas-Fermi distribution for the (sharp cutoff) momentum distribution (default);
= 3 ⇒ the same as 0, but using the (larger) nuclear radius of the Bertini model;
= 4 ⇒ the same as 1, but using the (larger) nuclear radius of the Bertini model;
= 5 ⇒ the same as 2, but using the (larger) nuclear radius of the Bertini model.
The corresponding ISABEL code input variable is IDEN, with default also 2.

l = 1 ⇒ reflection and refraction at the nuclear surface, but no escape cutoff for isobars;
= 2 ⇒ reflection and refraction at the nuclear surface, with escape cutoff for isobars;
= 3 ⇒ no reflection or refraction, with escape cutoff for isobars (default);
= 4 ⇒ the same as 1, but using a 25 MeV potential well for pions;
= 5 ⇒ the same as 2, but using a 25 MeV potential well for pions;
= 6 ⇒ the same as 3, but using a 25 MeV potential well for pions.
The corresponding input variable for the ISABEL code is MODEL = $l + 70$.

The default for ICHOIC is 23 (i.e., 0023); the defaults recommended for the ISABEL code would be represented by ICHOIC = 323. Not all the options for the ISABEL intranuclear cascade model have been thoroughly "debugged".

IFBRK 0 ⇒ use Fermi breakup model only for A $\leq$ 5; ⇐
1 ⇒ use Fermi breakup model for A $\leq$ 13 and for 14 $\leq$ A $\leq$ 20 with excitation below 44 MeV (default).

IPREQ 0 ⇒ no preequilibrium model will be used (default); ⇐
1 ⇒ use preequilibrium model following the intranuclear cascade [12] ;
2 ⇒ use IPREQ =1 and IPREQ = 3 randomly, with an energy-dependent probability that go to IPREQ = 3 at low incident energies and to IPREQ = 1 at high incident energies;
3 ⇒ use preequilibrium model *instead* of the intranuclear cascade.

Options IPREQ = 2 and IPREQ = 3 apply only when using the Bertini intranuclear cascade model (IEXISA = 0); when using the ISABEL model, these options default to IPREQ = 1.

ILVDEN -1 ⇒ use original HETC level density formulation; ⇐
0 ⇒ use Gilbert-Cameron-Cook-Ignatyuk level density model (default) [12];
1 ⇒ use the Jülich level density parameterization as a function of mass number [15].

JCOUL 1 ⇒ use Coulomb barrier on incident charged particle interactions (default) [16]; ⇐
0 ⇒ no Coulomb barrier for incident charged particles.

Record 5 List-directed with 10 data items.

NBERTP 1 ⇒ nucleon-pion transport only (default);
0 ⇒ muon transport only;
-1 ⇒ nucleon-pion-muon transport.
Other values are an error condition. The file BERTIN is required for NBERTP = ±1.

NELSTP 1 ⇒ neutron elastic scattering data read from input file; ⇐
0 ⇒ no neutron elastic scattering allowed (default for NOELAS = 0);
-1 ⇒ neutron elastic scattering data read from file ELSTIN (default for NOELAS > 0).

Applies only when neutron elastic scattering data is to be read in (NOELAS > 0); other values are an error condition (see Section 2.2).

⇒ **NEUTP** 0 ⇒ do not write NEUTP;
1 ⇒ write low energy neutrons to file NEUTP (default);
2 ⇒ write low energy neutrons and protons to file NEUTP;
3 ⇒ write low energy neutrons, protons, and deuterons to file NEUTP.
Other values are an error condition. Protons and deuterons may be written to source particle file NEUTP for subsequent transport with the multigroup option in HMCNP based on MCNP Version 3B [14].

NHSTP 1 ⇒ write history file HISTP (default); 0 ⇒ do not write HISTP. Other values are an error condition.

MXHIST Maximum number of history files to allow; the default is 27 and zero defaults to 27.
⇒ The absolute maximum number of history tapes is 27, with the naming sequence HISTP, HISTPA,...,HISTPZ. The run will terminate if MXHIST is exceeded. A test problem should be used to estimate the number of history files needed. If the estimate exceeds 27, the size of the files may be increased with LHIST, although the generation of many long files causes problems of files storage and retrieval. An alternative is to use IRECRD to limit the amount of data recorded in HISTP; obviously, data that is eliminated from HISTP cannot be available later for HTAPE analysis. *NOTE:* the maximum number of files is reduced if any files in the naming sequence are present in the local file space.

IRECRD 0 ⇒ use default record control to specify data to be put on history file;
1 ⇒ read records 5a and 5b to control the contents of the history file.
The default = 0; all other values are an error condition. The default mode excludes only multiple scattering subtrajectory records (NCOL = 8) and nucleon pseudo-collision records; these are rarely used except for debugging purposes. The remaining records are those necessary for a complete energy balance. All particles which are transported are included on the history file.

⇒ **NWSPRD** No longer used.

IEVAP 0 ⇒ the RAL evaporation-fission model will be used (default) [4];
1 ⇒ the ORNL evaporation-fission model will be used [3].
Other values are an error condition. The ORNL model allows fission only for isotopes with $Z \geq 91$.

NOFIS 1 ⇒ allow fission (default);
0 ⇒ suppress fission.
Other values are an error condition.

NOSKIP 0 ⇒ the next available random number is used to initiate a cascade;
> 0 ⇒ the random number is advanced 4297×NOSKIP each history.
The default is 10. Any value < 0 is an error condition. Using NOSKIP > 0 allows each history to start with a predetermined random number, allowing one to "inspect" a troublesome history in a subsequent run by using the JCASC parameter above. The purpose of using a large NOSKIP parameter is to prevent multiple use of the random number string between histories when many random numbers are generated per history.

Record 5a List-directed with 8 items (present only for IRECRD = 1).

KREC(I),I=1,8 0 ⇒ write records for NCOL = I;
1 ⇒ suppress records for NCOL = I.

The definition of the record types NCOL are given in Table 2.1. For more details about HISTP, see Appendix C.

NCOL	record type
1	source
2	nuclear interaction (secondaries from cascade)
3	charged particle slowed to cutoff
4	escape from system
5	pseudo-collision
6	nuclear absorption (no secondaries from cascade)
7	internal boundary crossing
8	multiple scattering subtrajectory

Table 2.1: HISTP Record Types

Record 5b List-directed with (up to) 18 items (present only for IRECRD = 1).

KPART(I),I=1,18 0 ⇒ write records for particle index I;
1 ⇒ suppress records for particle index I.

A list of the particle indices is given in Table 2.2. Note that the $\pi^0$and photon do not cause any HISTP records to be written, so that whether KPART(4) or KPART(12) is 1 or 0 is immaterial.

Record 6 List-directed with 10 items.

NSPRED 0 ⇒ multiple Coulomb scattering neglected;
> 0 ⇒ calculate multiple scattering for primary charged particles.
The default is 1; NSPRED < 0 or NSPRED > 5 is an error condition. For NSPRED > 1, the default step size for the multiple scattering treatment is reduced by a factor of 1/NSPRED.

NEXITE 1 ⇒ subtract nuclear recoil energy to obtain nuclear excitation energy (default);
0 ⇒ do not subtract nuclear recoil energy.
Other values are an error condition. See [1] for a discussion.

NPIDK 1 ⇒ force $\pi^-$to terminate by decay at the pion cutoff energy;
0 ⇒ force $\pi^-$to interact by intranuclear cascade when cutoff is reached (default).
Other values are an error condition.

N1COL 1 ⇒ compute cascade histories only through the second generation;
0 ⇒ compute all generations (default);
-1 ⇒ compute nuclear interactions of source particles only.
Other values are an error condition. For N1COL = -1, transport and slowing-down are turned off. Only nuclear interaction records are written to HISTP (NCOL=2 and NCOL=6). The interaction occurs in the first material of the problem; any other material specified is not used in the problem. This option is useful in calculating cross sections using the XSEX code to process HISTP. When using this option, it may be desirable to set the total atom density in the material to 1.0 so that XSEX will produce cross sections directly in barns. *At the present time, particle types 13. to 18. may only be used with* NCOL = -1.

LTME No longer used. ⇐

NLEDIT 1 ⇒ print out edit of neutron elastic scattering data;
0 ⇒ no such edit (default).
Other values are an error condition; relevant only if NOELAS > 0 (see Section 2.2).

Index	Type	Particle
1	0.	proton
2	1.	neutron
3	2.	π^+
4	3.	π^0
5	4.	π^-
6	5.	μ^+
7	6.	μ^-
8	7.	deuteron
9	8.	triton
10	9.	^{3}He
11	10.	alpha
12	11.	photon
13	12.	K^+
14	13.	K^0long
15	14.	K^0short
16	15.	K^-
17	16.	$\bar{p}$
18	17.	$\bar{n}$

Table 2.2: Particle Type Identification

NLRNGE 1 ⇒ print range-energy tables for charged particles;
0 ⇒ no such edit (default).
Other values are an error condition.

ISRFSR 1 ⇒ read surface source from file HISTIN;
0 ⇒ use default source or user-supplied source (default).
Other values are an error condition.

ICPT 1 ⇒ transport heavy charged particles;
0 ⇒ do not transport heavy charged particles.
The default is 0 for IEXISA = 0; the default is 1 for IEXISA $\geq$ 1. Other values are an error
⇒ condition. With this option, deuterons, tritons, ^{3}He's, and alphas may be transported; however, nuclear interactions are included only with the ISABEL intranuclear cascade model.

NOBAL 0 ⇒ use mass-energy balancing in the cascade and evaporation stages;
1 ⇒ turn off mass-energy balancing in the cascade stage;
2 ⇒ turn off mass-energy balancing in the evaporation stage;
3 ⇒ turn off mass-energy balancing in the cascade and evaporation stages.
⇒ The default is 1; other values are an error condition. Previous versions of HETC used a default of 0; however, a forced energy balance distorts the intent of either intranuclear cascade model; the user should explore the effect of energy balancing, utilizing HTAPE with option 7. Energy balancing for the intranuclear cascade is controlled by input parameter FLIM0 below.

Record 7 List-directed with 15 items, all floating point.

EMAX The maximum energy for particles in MeV. The default is 3495 MeV and zero defaults to 3495 MeV. For the Bertini INC model there is no upper limit on EMAX, although the

scaling law model used to extrapolate the Bertini model above 3.5 GeV gets unrealistic above 10 GeV. For the ISABEL INC model, the practical upper limit is 1000 MeV (or 1000 ⇐ MeV per nucleon for composite particles).

ELOP The low energy cutoff for protons in MeV (and heavier charged particles if they are tracked). *However, if protons and deuterons are to be recorded on file NEUTP using options NEUTP = 2 or 3, then their cutoff energy is determined by ELON below.* The default is 1 ⇐ MeV; anything less defaults to 1 MeV.

ELON The low energy cutoff for neutrons in MeV, and for protons and deuterons when they are to be written to file NEUTP. The default is 20 MeV; zero defaults to 20 MeV. Neutrons (and ⇐ perhaps protons and deuterons, according to the value of input parameter NEUTP above) appearing with energy less than ELON are recorded on the source particle file NEUTP for subsequent transport with a Monte Carlo code such as HMCNP.

EPICUT The low energy cutoff for pions in MeV. The default is 0.149 MeV; anything less takes the default.

EMUCUT The low energy cutoff for muons in MeV. The default is 0.113 MeV; anything less takes the default.

CTOFE The cutoff energy (MeV) for particle escape during the intranuclear cascade *when using the Bertini model.* The cutoff energy prevents low energy nucleons from escaping the nucleus during the intranuclear cascade; for protons, the actual cutoff is the *maximum* of CTOFE and a Coulomb barrier. For CTOFE $\geq$ 0, CTOFE will be used as the cutoff energy. For CTOFE $<$ 0, a *random* cutoff energy, uniformly distributed from zero to twice the mean binding energy of a nucleon, will be sampled for each projectile-target interaction and separately for neutrons and protons; in this case, the Coulomb barrier for protons is also randomized. *The randomized cutoff energy is the default procedure;* i. e. CTOFE = -1 ⇐ is the default value. For the ISABEL INC, the randomized cutoff energy is always used.

ELAS The high energy cutoff for neutron elastic scattering with nuclei other than ^{1}H. The default is 50 MeV, zero defaults to 50 MeV and the maximum is 100 MeV. The value of ELAS is pertinent only for NOELAS $>$ 0 (see Section 2.2), in which case it must be below the maximum energy for which the data is provided.

WTPI The minimum weight for pions. The default is 0.1; zero or negative takes the default. If WTPI $<$ WTMU, WTPI is set equal to WTMU. If the pion weight falls below WTPI, decay is allowed only by an analog process.

WTMU The minimum weight for muons produced by pion decay. The default is 0.1 and zero or negative takes the default. If WTMU equals 1, or if the pion weight is less than WTMU, pion decay is described by an essentially analog process. If WTMU $<$ 1, more than one muon track may be produced per pion decay; on the average, 1/WTMU tracks for the decay of a weight 1 pion will be created.

FLIM0 The maximum correction allowed for mass-energy balancing in the cascade stage, used with NOBAL = 1 and NOBAL = 3. For FLIM0 $>$ 0, kinetic energies of secondary particles will be reduced by no more than a fraction of FLIM0 in attempting to obtain a non-negative excitation of the residual nucleus and a consistent mass-energy balance; a cascade will be resampled if the correction exceeds FLIM0. For FLIM0 = 0, no correction will be attempted and a cascade will be resampled if a negative excitation is produced. For FLIM0 $<$ 0 (default), a default procedure is used in which the maximum correction is 0.02 for incident energy above 250 MeV, 0.05 for incident energy below 100 MeV, and is set equal to 5/(incident energy) between those limits.

YZERE The Y0 parameter in the level density formula for $Z \leq 70$. The default is 1.5; zero or negative is an error condition. For target nuclei with $Z \leq 70$, the parameters BZERE and YZERE are used to compute level densities; the default values are those used in LAHET before installation of the ORNL fission model. For target nuclei with $Z \geq 71$, the BZERO and YZERO parameters are used to compute level densities for the target nucleus and the fission fragments. To be consistent with current ORNL practice, BZERE should be set equal to 10.0 in any problem in which fission is allowed (IEVAP = 1). *Applies only for ILVDEN = -1.*

⇒

BZERE The B0 parameter in the level density formula for $Z \leq 70$. The default is 8.0; zero or negative is an error condition (see YZERE above). *Applies only for ILVDEN = -1.*

⇒

YZERO The Y0 parameter in the level density formula for $Z \geq 71$ and all fission fragments. The default is 1.5; zero or negative is an error condition (see YZERE above). *Applies only for ILVDEN = -1.*

⇒

BZERO The B0 parameter in the level density formula for $Z \geq 71$ and all fission fragments. The default is 14.0 for IEVAP = 0 and is 10.0 for IEVAP = 1; zero or negative is an error condition (see YZERE above). *Applies only for ILVDEN = -1.* The results of experiments run at LANL's WNR facility indicate that it is desirable to use BZERO = 8.0 with IEVAP = 0 for proton beams of energy below 1 GeV.

⇒

SWTM 0 ⇒ low-energy particles are written to file NEUTP unmodified;
> 0 ⇒ a roulette scheme is used for any particle with weight WT < SWTM.
The default is 0.0; negative values are an error condition. If the particle weight WT < SWTM, the particle is killed with probability (1-WT/SWTM); otherwise, it is kept and given the weight SWTM. This option may be used to reduce the number of particles placed on the NEUTP file for subsequent HMCNP tracking.

Record type 8 List-directed with 3 items. For each medium M = 1,...,MXMAT, include one type 8 record followed by one or more type 9 records as needed.

DENH(M) Hydrogen (^{1}H) density in medium M, atoms/cubic Angstrom; the default is 0.

NEL(M) The number of nuclides other than ^{1}H in medium M. There is no default and at least one isotope other than ^{1}H must be entered with a non-zero, albeit infinitesimal, density. The maximum is 30.

NOEL(M) The number of nuclides in medium M (other than ^{1}H) for which neutron elastic scattering is to be included. The default is 0 and the maximum is NEL(M).

Record type 9 List-directed with 4 items. One type 9 record appears for each L, L=1,NEL(M).

ZZ(L,M) The charge number of the Lth nuclide in the Mth medium (no default).

A(L,M) The mass number of the Lth nuclide in the Mth medium (no default). *Warning:* this is the mass number, ***not the atomic weight***; a non-integral value will cause errors.

DEN(L,M) The atom density (atoms per cubic Angstrom) of the Lth nuclide in the Mth medium (no default); it must be greater than zero.

ID(L,M) The position of data for nuclide (L,M) in the neutron elastic scattering data input. See Section 2.2. The default is 0; zero means no data. The maximum is NOELAS.

Record types 1 through 9 may be followed, in order, by the following blocks of data:

ID	Z	A		ID	Z	A
1	3	6		13	26	56
2	3	7		14	29	63
3	4	9		15	40	90
4	5	10		16	42	98
5	6	12		17	47	107
6	7	14		18	50	120
7	8	16		19	64	158
8	13	27		20	74	184
9	14	30		21	79	197
10	16	32		22	82	208
11	22	48		23	92	238
12	24	52				

Table 2.3: Contents of File /LCS/ELSTIN

- Neutron elastic scattering data - present if NOELAS > 0 and NELSTP = 1 (see Section 2.2 and Appendix E).
- Geometry data - at present, only MCNP geometry is available (see Section 2.3).
- Source routine data - as required by a user-supplied source; for input required by the default source, see Section 2.4.

2.2 NEUTRON ELASTIC SCATTERING DATA

The user may specify neutron elastic scattering for any isotope in the problem for neutron energies below 100 MeV. The scattering algorithm is a very simplified one which preserves only the first moment $\bar{\mu}$, where μ is the scattering angle in the center of mass. The sampled probability distributions are given by

$$P(\mu) = \frac{1}{2} + \frac{3\bar{\mu}\mu}{2} \text{ for } -1/3 < \bar{\mu} < 1/3$$

$$P(\mu) = \frac{3(1-\bar{\mu})(\mu+1)}{4} + \frac{(3\bar{\mu}-1)\delta(\mu-1))}{2} \text{ for } 1/3 < \bar{\mu} < 1$$

$$P(\mu) = \frac{3(1+\bar{\mu})(1-\mu)}{4} - \frac{(3\bar{\mu}+1)\delta(\mu+1))}{2} \text{ for } -1 < \bar{\mu} < -1/3$$

where δ is the Dirac function.

To invoke neutron elastic scattering, the user must supply a library of tabulations of the elastic cross section σ_{el} and the mean center of mass scattering cosine $\bar{\mu}$ as a function of incident lab energy. The data may be read from file ELSTIN (NELSTP = -1) or inserted into the INH file as described above (NELSTP = 1). In either case, the data is supplied in BCD with the format discussed in Appendix E. The variable NOELAS is the number of isotopic data tabulations in the supplied library and ELAS is the maximum energy at which elastic scattering may be used. The variable ID for each isotope on record type 9 represents the sequential position of the data which are to be used for that isotope

among the NOELAS tabulations. Since data may not be available for every isotope in the problem, it is generally reasonable to reference the data for an isotope near in mass.

To encourage exploration and testing of the neutron elastic scattering option, a default ELSTIN ⇒ file has been generated and is available from CFS as "**/LCS/ELSTIN**." The contents of the files are listed in Table 2.3, along with the appropriate values of ID needed to reference the data. The data were generated with the SCAT79 optical model code using the Becchetti-Greenlees potential. The data are tabulated on a 9-point energy grid from 10 MeV to 50 MeV. When using the default ELSTIN file, use NOELAS = 23, NELSTP = -1, and ELAS = 50.

2.3 MCNP GEOMETRY INPUT

The geometry input for the current operational version of LAHET is described in the older MCNP manual[2]. All features of the MCNP geometry capability are included in LAHET at the level of MCNP version 2D. The structure of the geometry input is as follows:

cell records
one blank line
surface records
one blank line
IN importance record
PRINT record (optional)
one blank line.

The only required MCNP data record is the cell importance (IN) record. Note that the designation of cell importance records has changed in recent versions on MCNP; however, the IN record must be used in the LAHET input. The PRINT record may also be used, and is recommended. Other MCNP input records at the level of MCNP version 2D may be included in the input file and will be ignored; MCNP input record types which have been introduced in versions 3, 3A, and 3B ([13],[14]) may cause an error and should be avoided. *Note:* the material densities on the MCNP cell cards are *not* used by LAHET; the atom densities are taken from the type 9 records described above. *Warning:* since LAHET uses the "list-directed input" described in Chapter I, the slash "/" may not be used on any MCNP geometry record *except* where it is a part of the surface type designator.

Since geometric splitting is not available in this version, the only significance to the values entered on the IN record is whether a zero or a non-zero value appears. A zero indicates an external void (a leakage cell or black absorber) and a non-zero value is replaced by unity.

The maximum number of cells or surfaces that may be input is 450 in the present version.

2.4 LAHET DEFAULT SOURCE OPTIONS

2.4.1 Source Specification

To specify one of the allowed default source options, at least the following record must be supplied. It is in list-directed format with up to 10 data items.

ISOPT -1 ⇒ An *isotropic* point source in the (x,y)-plane; ⇐
0 ⇒ A parallel beam uniformly distributed over an ellipse (default);
1 ⇒ A parallel beam with parabolic density over an ellipse;
2 ⇒ A parallel beam with Gaussian density over an ellipse;
3 ⇒ A parallel beam elliptical ring source with user-supplied density distribution;
4 ⇒ A parallel beam uniformly distributed in a rectangle;
9 ⇒ The same as ISOPT = -1 with input energy distribution;
10 ⇒ The same as ISOPT = 0 with input energy distribution;
11 ⇒ The same as ISOPT = 1 with input energy distribution;
12 ⇒ The same as ISOPT = 2 with input energy distribution;
13 ⇒ The same as ISOPT = 3 with input energy distribution;
14 ⇒ The same as ISOPT = 4 with input energy distribution.

E0 The source energy in MeV; the default is 800 MeV. For the parallel beam sources, the *sign* applied to E0 is relevant. If a negative value for E0 is entered, the source particles are emitted in the negative z-direction and the absolute value of E0 is used as the source energy; otherwise, the source is emitted in the positive z-direction. E0 applies only to ISOPT = -1,...,4.

TIP0 The source particle type in floating point from Table 2.2. The default is 0.0 (proton). Nucleons and charged pions will interact when transported using either intranuclear cascade model. Muons will slow down and decay without nuclear interaction. The ion types 7. through 10. will interact using the ISABEL model, but will only slow down otherwise. Antinucleons and kaons may be ⇐ used for a cross section interaction calculation (N1COL=-1) only, since provision for transporting kaons has not yet been implemented. Photons and π^0's may not be input as source particles.

Z0 The starting z-coordinate for the source (the default is 0.0). A value of Z0 should be selected such that the source *does not coincide exactly with a plane* separating two cells; a very small shift in the beam direction will suffice. If the source is coincident exactly with a plane separating an importance 1 cell from an importance 0 cell, histories will be lost since some source particles will be born in an external void region. (A warning of this condition is printed out in file OUTH). In other cases, tracking errors may occur.

A0 The semi-major axis parameter. The default is 0.0; a value of 0.0 will produce a "pencil beam" source. For ISOPT = 4 or 14, A0 is the rectangular half-length along the x'-axis. To understand the option-dependent definition of A0, the user *must* read the following section.

B0 The semi-minor axis parameter. The default is A0; if B0 = A0, a circular (or square) source will be produced. For ISOPT = 4 or 14, B0 is the rectangular half-length along the y'-axis. *NOTE*: for the *elliptical* sources (ISOPT = 0, 1, 2, 3, 10, 11, 12, or 13) B0 $\leq$ A0 is *required*. To understand the option-dependent definition of B0, the user *must* read the following section.

CUTS The cutoff parameter used with ISOPT = 1, 2, 11, or 12. The default is 1.0 for ISOPT = 1 or 11 and is 3.717 for ISOPT = 2 or 12; in either case, zero takes the default. CUTS is not used for ISOPT = -1, 0, 3, 4, 9, 10, 13, or 14. For ISOPT = 1 or 11, CUTS should be between 0 and 1; CUTS = 1.0 is the same as no cutoff at all. For ISOPT = 2 or 12, any positive value is allowed. To understand the use of CUTS, the user must read the following section with particular attention to equations 2.3 and 2.4.

SMU The cosine of rotation of the source ellipse or rectangle (the default is 0.0). SMU is immaterial for A0 = B0 unless ISOPT = 4 or 14). To fully understand the definition and use of SMU,

the user must carefully read the following section and understand the transformation given by equations 2.1 and 2.2. Note that SMU = 0.0 implies no transformation at all.

X0 The x-coordinate for the center of the source distribution (the default is 0.0).

Y0 The y-coordinate for the center of the source distribution (the default is 0.0).

For ISOPT = 3 or 13, the following two additional records must be supplied; each is in list-directed format and may contain up to 100 entries.

SRING2(I),I=1,NRING Ring boundary parameters for NRING elliptical rings in increasing order.

SPROB(I),I=1,NRING Ring probability values for NRING elliptical rings. They need not be normalized.

The items of the above two records must be in a one-to-one correspondence. The function of ISOPT = 3 or 13 is described below.

To specify a probability distribution for the source particle energy with ISOPT = 9, 10, 11, 12 or 13, two records must be supplied which may have up to 200 entries.

ESRC(I),I=1,NEPRB Energy bin boundaries for NEPRB-1 energy bins, within each of which the source energy will be uniformly sampled.

EPRB(I),I=1,NEPRB Probability specification for sampling from the NEPRB-1 energy bins, in either of the two forms described below.

The EPRB array may be entered *either* as the unnormalized energy probability density value times the bin width for each energy bin *or* as the corresponding cumulative source energy distribution values. In either case, EPRB(1) *must be* 0. The cumulative distribution method is determined by the fact that the last EPRB entry must be *precisely unity*; consequently, when using the first method, the last EPRB entry must not be unity. As an example, consider the energy probability table entered as

```
100.,200.,400./
0.,6.,4./
```

In this case, the source energy bin from 100 MeV to 200 MeV will be sampled 60% of the time and the bin from 200 MeV to 400 MeV will be sampled 40% of the time. The same distribution entered using the cumulative density method would use the records

```
100.,200.,400./
0.,.6,1./
```

In either case, the probability density in the first bin is 0.006/MeV and in the second is 0.002/MeV.

If desired, the user may add a record after the above spatial source description to assign a time dependence to the source pulse. The source time record is list-directed with 4 data items and has the form "**ITOPT,TWIT,TPEAK,TSIG/**".

ITOPT -1 ⇒ Set the source time to TPEAK (default);
- 0 ⇒ Sample the source time from a uniform distribution of width TWIT centered at TPEAK.
- 1 ⇒ Sample the source time from a parabolic distribution of width TWIT centered at TPEAK.
- 2 ⇒ Sample the source time from a Gaussian distribution of standard deviation TSIG centered at TPEAK with width TWIT.
- 3 ⇒ Sample the source time from a user-input probability table.

TWIT The source pulse width in nanoseconds (the default is 0).

TPEAK The pulse center in nanoseconds (the default is 0).

TSIG The standard deviation of a Gaussian pulse (the default is TWIT/4).

The parameters TWIT and TPEAK are meaningful only for ITOPT = 0, 1, or 2; TSIG is meaningful only for ITOPT = 2. For ITOPT = 3, the following two records, with up to 200 entries each, must be supplied to give the source time probability distribution.

TSRC(I),I=1,NTPRB Time bin boundaries for NTPRB-1 time bins, within each of which the source time will be uniformly sampled.

TPRB(I),I=1,NTPRB Probability specification for sampling from the NTPRB-1 time bins.

The methods for entering (and sampling from) the TSRC and TPRB arrays is exactly the same as for the ESRC and EPRB arrays described above. TPRB(1) *must be* 0.

2.4.2 Spatial Distribution of the Source

To illustrate the properties of the various source options, let us make the following definitions:

$$x_0 \equiv \mathrm{X0} \qquad y_0 \equiv \mathrm{Y0}$$

$$a \equiv \mathrm{A0} \qquad b \equiv \mathrm{B0}$$

$$c \equiv \mathrm{CUTS}$$

$$\cos\phi \equiv \mathrm{SMU}$$

where $\sin\phi \geq 0$. The source is generated in an (x', y') coordinate system with the distribution centered at the origin and the major axis of the distribution along the positive x'-direction. The particle coordinates are then obtained by translation and rotation according to the following equations:

$$x = x' \sin\phi - y' \cos\phi + x_0 \quad , \tag{2.1}$$

$$y = x' \cos\phi + y' \sin\phi + y_0 \quad . \tag{2.2}$$

Thus angle ϕ is the angle of rotation of the major axis of the source distribution from the positive y-direction in the laboratory coordinate system. For the default SMU = 0.0, the angle ϕ is 90° and the major axis lies along the x-axis. A rotation cosine SMU may be used with any source option except the point source.

For ISOPT = -1 or 9, $x' \equiv 0$ and $y' \equiv 0$ so that $x \equiv x_0$ and $y \equiv y_0$. Otherwise, the distribution of (x', y') values is given by the appropriate probability density function $p(x', y')$.

For ISOPT = 0 or 10, the source distribution is uniform in an ellipse defined by

$$\left(\frac{x'}{a}\right)^2 + \left(\frac{y'}{b}\right)^2 \leq 1 \quad .$$

Consequently,

$$p(x', y') = \frac{1}{\pi a b} \quad .$$

The CUTS parameter is not used.

For ISOPT = 1 or 11, the source has a parabolic distribution with a probability density given by

$$p(x',y') = \frac{2}{\pi abc(2-c)}\left[1-\left(\frac{x'}{a}\right)^2-\left(\frac{y'}{b}\right)^2\right]$$

and vanishing outside of the ellipse defined by

$$\left(\frac{x'}{a}\right)^2+\left(\frac{y'}{b}\right)^2 \le c \quad . \tag{2.3}$$

In the laboratory system, the distribution is entirely confined within a circle of radius $a\sqrt{c}$ centered at (x_0, y_0).

For ISOPT = 2 or 12, the source has a Gaussian distribution and is sampled from a density function given by

$$p(x',y') = \frac{\exp\left[-\frac{1}{2}\left[\left(\frac{x'}{a}\right)^2+\left(\frac{y'}{b}\right)^2\right]\right]}{2\pi ab\left[1-\exp\left(\frac{-c^2}{2}\right)\right]} \quad .$$

The source vanishes outside the ellipse given by

$$\left(\frac{x'}{a}\right)^2+\left(\frac{y'}{b}\right)^2 \le c^2 \tag{2.4}$$

and, in the laboratory system, this elliptical region is entirely confined within a circle of radius ac centered at (x_0, y_0). Note that the cutoff parameter CUTS is specified as a multiple of standard deviations of the Gaussian distribution. The default value of 3.717 implies that $p(x',y') = 10^{-6}$ on the boundary of the distribution.

For ISOPT = 3 or 13, the user defines a sequence of nested elliptical rings, using the A0, B0, and SRING2 parameters, and the probability SPROB(I) of sampling the source point *uniformly* within a ring. Let us make the following definitions:

$$P_i \equiv \text{SPROB(I)} \qquad f_i \equiv \text{SRING2(I)} \qquad f_0 \equiv 0 \quad .$$

Then an elliptical ring i is defined by

$$f_{i-1}^2 \le \left(\frac{x'}{a}\right)^2+\left(\frac{y'}{b}\right)^2 \le f_i^2 \quad ;$$

af_i and bf_i are the semi-major and semi-minor axes of the outer boundary, while af_{i-1} and bf_{i-1} are the semi-major and semi-minor axes of the inner boundary of the elliptical ring. The probability of sampling an (x', y') point within ring i is then given by probability P_i. Within ring i, the sampling is uniform, with probability density given by

$$p_i(x',y') = \frac{1}{\pi ab(f_i^2-f_{i-1}^2)} \quad .$$

The sampled point is then translated and rotated from the (x', y') frame into the (x, y) frame. The probability P_i of any interior ring may be 0.0 to produce a two-dimensional "doughnut" source.

For ISOPT = 4 or 14, the point (x', y') is obtained by uniformly sampling in the rectangle given by

$$-a \le x' \le +a \qquad -b \le y' \le +b$$

and translated and rotated into (x, y) as above. In particular, the probability density function is just

$$p(x', y') = \frac{1}{4ab}$$

within the rectangle and is 0 without.

2.4.3 Time Distribution of the Source

To characterize the time distribution options, let us make the following definitions.

$$t_p \equiv \text{TPEAK} \quad \Delta t \equiv \text{TWIT} \quad \sigma \equiv \text{TSIG} \quad .$$

- For ITOPT = -1, $t = t_p$ is always assigned.
- For ITOPT = 0, the source time t is sampled from the uniform distribution

$$p(t) = \frac{1}{\Delta t} \quad \text{for} \quad t_p - \frac{1}{2}\Delta t \leq t \leq t_p + \frac{1}{2}\Delta t \quad ;$$

$$p(t) = 0 \quad \text{otherwise.}$$

- For ITOPT = 1, the source time t is sampled from the parabolic distribution

$$p(t) = \frac{3}{2\Delta t}\left[1 - \left(\frac{2(t - t_p)}{\Delta t}\right)^2\right] \quad \text{for} \quad t_p - \frac{1}{2}\Delta t \leq t \leq t_p + \frac{1}{2}\Delta t \quad ;$$

$$p(t) = 0 \quad \text{otherwise.}$$

- For ITOPT = 2, the source time is sampled form the truncated Gaussian distribution

$$p(t) = \frac{1}{\sqrt{2\pi}\sigma \operatorname{erf}\left(\frac{\Delta t}{2\sqrt{2}\sigma}\right)} \exp\left[-\frac{(t - t_p)^2}{2\sigma^2}\right] \quad \text{for} \quad t_p - \frac{1}{2}\Delta t \leq t \leq t_p + \frac{1}{2}\Delta t \quad ;$$

$$p(t) = 0 \quad \text{otherwise.}$$

- For ITOPT = 3, the source time is sampled from the input probability table. Define

$$P_i \equiv \text{TPRB(I)} \quad ; \quad t_i \equiv \text{TSRC(I)} \quad .$$

  P_i is the probability for selecting the source time in the interval $t_{i-1} \leq t \leq t_i$ for i = 2,...,NTPRB; within the interval, the sampling is uniform.

2.5 EXECUTING LAHET

The executable file is named LAHET. The input file version is designated by INH; it may be defined by file replacement. If NBERTP = ±1, the file BERTIN is required. If NOELAS > 0 and NELSTP = -1, elastic scattering data file ELSTIN is required.

The files LAHET, BERTIN, and ELSTIN are on the Common File System under the node "/LCS". The essential execute lines are

```
MASS GET DIR=/LCS LAHET BERTIN ELSTIN
LAHET INH=user-file / t v
```

The output files produced by LAHET are the printer output, OUTH, the history file HISTP and its continuations HISTPA, HISTPB, etc., and the neutron source file NEUTP and its continuations NEUTPA, NEUTPB, etc. If a file with one of these names is already present in the local file space, the new file will be given the next name available in the sequence (e.g., if OUTH is already present, the new printer output file will be given the name OUTHA). All input and output files may be assigned to new names using file replacement on the execute line.

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Chapter 3

THE HTAPE CODE

3.1 INPUT FOR HTAPE

HTAPE is the code designed to provide analysis of the history file written by LAHET. In its latest version, it has been modified to process a leakage neutron file produced by HMCNP, the LAHET-compatible version of MCNP. The various edit options and the required input are described in this section. In general, energy units are MeV, time units are nanoseconds, and length units are centimeters.

The input file (default name INT) for HTAPE has the following structure:

1. Two records of title information, 80 columns each.
2. An option control record.
3. Additional input as required by the chosen option.

Items 2 and 3 above are written as "list-directed input" described in Chapter 1. Repeat counts are allowed, including repeat counts for commas to take default values (i.e., "4*," expands to ",,,,"). Multiple cases may be processed; for each case the above structure applies. Slashes "/" are allowed *only* in the first pair of title cards *unless* each title card containing one or more slashes has a " $ " in column 1.

The option control record defines the options to be used and the additional input information that must be specified for the problem. The structure of this record is

IOPT,NERG,NTIM,NTYPE,KOPT,NPARM,NFPRM,FNORM,KPLOT,IXOUT,IRS, IMERGE,ITCONV,IRSP/

Some of the parameters in this record may optionally be preceded by a minus sign whose meaning is defined below (see Table 3.2 for applicability). Thus if NTIM is specified by inserting "-3" in the option control record, it is interpreted as NTIM = 3 with a *minus-sign flag* attached. In the discussion which follows, input control parameters are treated as positive or zero quantities, even though the flag may be present.

IOPT defines the editing option to be applied. At the present time, IOPT = 1, . . . ,14 are the allowed basic option types as defined below. For all but IOPT = 7 or 13, one may add 100 to the basic option type to indicate that the tally over a list of cell, surface, or material numbers will be combined in a single tally. Prefixing IOPT by a minus sign, when allowed, indicates an option-dependent modification to the tally.

IOPT	NERG	NTIM	NTYPE	NPARM	NFPRM	KPLOT	IXOUT	IMERGE	ITCONV	IRSP
1	O	O	R	O	O	N	N	O	O	O
101	O	O	R	R	O	N	N	O	O	O
2, 102	O	O	R	R	N	N	N	O	O	O
3	O	O	N	O	N	O	N	N	O	N
103	O	O	N	R	N	O	N	N	O	N
4, 104	O	N	N	R	N	N	N	N	N	O
5	N	N	N	O	N	O	N	N	N	N
105	N	N	N	R	N	O	N	N	N	N
6	N	O	N	O	N	N	N	N	O	N
106	N	O	N	R	N	N	N	N	O	N
7	N	N	N	O	N	N	N	N	N	N
8	N	N	N	O	N	O	O	N	N	N
108	N	N	N	R	N	O	O	N	N	N
9, 109	O	O	R	R	O	N	N	O	O	O
10, 110	O	O	R	R	N	N	N	O	O	O
11, 111	O	N	R	R	O	N	N	O	N	N
12, 112	O	N	R	R	O	N	N	O	N	N
13	O	O	R	O	O	N	N	O	O	O
14	N	N	N	O	N	N	N	N	N	N
114	N	N	N	R	N	N	N	N	N	N

R ≡ required O ≡ optional N ≡ not used
IRS is optional with any value of IOPT

Table 3.1: Applicability of Input Control Parameters

NERG, when applicable, defines the number of energy bins for the tally; the maximum is 2000. The default is 0, implying that only a total over energy will be produced. If NERG is > 1 and is preceded by a minus sign, the tally in each energy bin will be divided by the bin width to normalize per MeV. The total over energy will be unnormalized.

NTIM defines the number of time bins for the tally when applicable; the maximum is 100. The default is 0, implying that only a total over time will be produced. If NTIM is > 1 and is preceded by a minus sign, the tally in each time bin will be divided by the bin width to normalize per nanosecond; the total over time will be unnormalized.

NTYPE defines the number of particle types for which the edit is to be performed for those options where it is applicable; the particle type is that of the particle causing the event which is recorded on the history tape. The default is 0; however, some options require that a value be supplied.

KOPT defines a sub-option for tally option IOPT. The default is 0.

NPARM *usually* defines the number of cells, materials, or surfaces over which the tally is to be performed when applicable; the maximum is 400. If NPARM is preceded by a minus sign, NPARM+1 normalization divisors will be read in as described below. The default is 0; however, some options require that a value be supplied.

IOPT	-IOPT	-NERG	-NTIM	-NTYPE	-NPARM	-NFPRM
1, 101	O	O	O	N	O	O
2, 102	O	O	O	N	O	N
3, 103	O	O	O	N	O	N
4, 104	O	O	O	N	O	N
5, 105	O	N	N	N	O	N
6, 106	N	N	N	N	O	N
7	N	N	N	N	O	N
8, 108	O	N	N	N	O	N
9, 109	O	O	O	N	O	O
10, 110	O	O	O	N	O	N
11, 111	N	O	N	N	O	O
12, 112	N	O	N	N	O	O
13	O	O	O	N	N	N
14, 114	N	N	N	N	O	N

O ≡ optional N ≡ not used

Table 3.2: Applicability of Minus-sign Flags on Input Control Parameters

NFPRM, at present, is used only to define the number of cosine bin boundaries to read in for particle current tallies; the maximum is 400. If NFPRM is preceded by a minus sign, cosine bin tallies will be normalized per steradian: the total over cosine bins will remain unnormalized (i.e., angle integrated). The default is 0.

FNORM may be used to apply an overall multiplicative normalization to all bins, except for IOPT = 11, 111, 12, or 112. For these cases, FNORM multiplies the time variable (e.g., use FNORM = 0.001 to convert from nanoseconds to microseconds). The default is 1.0.

KPLOT is a plot control flag; plotting is available for some options. Using a 0 indicates that no PLOT file will be produced and is the default.

IXOUT is a flag to indicate that the tally will be written to a formatted auxiliary output file for post-processing. The details (and the file name) are option dependent; however, a 0 indicates that no such file will be written, and is the default.

IRS is the RESOURCE option flag. A non-zero value indicates that the option will be turned on; 0 is the default (see Section 3.3 below).

IMERGE is the file combination (MERGE) option flag. A non-zero value indicates that *both* a HISTP and a HISTX will be simultaneously edited to produce a common tally; 0 is the default. Since at the present time a HISTX file can contain only surface crossing records (NCOL = 7), this feature is meaningful only when the basic option type is 1, 2, 9, 10, 11, 12, or 13 (see Section 3.4 below).

ITCONV is the TIME CONVOLUTION option flag. A non-zero value indicates that the option will be turned on; 0 is the default (see Section 3.5 below). ⇐

(-)IOPT, . . .	option control record (always required)
ERGB(I),I=1,NERG	upper energy bin limits
TIMB(I),I=1,NTIM	upper time bin limits
ITIP(I),I=1,NTYPE	particle type identifiers
LPARM(I),I=1,NPARM	surface, cell, or material identifiers
FPARM(I),I=1,NFPRM	upper cosine bin boundaries
DNPARM(I),I=1,NPARM+1	normalization divisors
	original source definition record for RESOURCE option
	new source definition record for RESOURCE option
ITOPT,TWIT,TPEAK,TWIT	parameters for TIME CONVOLUTION
ERESP(I),I=1,NRESP	energy grid for RESPONSE FUNCTION
FRESP(I),I=1,NRESP	function values for RESPONSE FUNCTION
IRESP(I),I=1,NRESP-1	interpolation scheme for RESPONSE FUNCTION
	segment definition record or window definition record
CN(I),I=1,3	arbitrary direction vector for defining cosine binning

Table 3.3: Order of HTAPE Input Records

IRSP is the RESPONSE FUNCTION option flag. IRSP > 0 indicates that the tally will be *multiplied* by a user-supplied response function; IRSP < 0 indicates that the tally will be *divided* by a user-supplied response function. The default is 0. For a discussion, see Section 3.6 below.

The standard definitions for these input variables may not apply for some options. The applicability of the option control parameters is summarized in Table 3.1.

According to the parameters specified on the option record, the following records are required in the order specified:

- For NERG > 0, a record defining NERG upper energy bin boundaries, from low to high, defined as the array ERGB(I),I=1,NERG. The first lower bin boundary is implicitly always 0.0. The definition may be done in four different ways. First, the energy boundary array may be fully entered as ERGB(I), I=1,NERG. Second, if two or more, but less than NERG, elements are given (with the record terminated by a slash), the array is completed using the spacing between energy boundaries obtained from the last two entries. Third, if only one entry is given, it is used as the first upper energy boundary and as a constant spacing between all the boundaries. Fourth, if only two entries are given with the first negative and the second positive, the second entry is used as the uppermost energy boundary, ERGB(NERG), and the first entry is interpreted as the lethargy spacing between bin boundaries. Thus the record "**-0.1,800./**" will specify ten equal-lethargy bins per decade from 800 MeV down.

- For NTIM > 0, a record specifying NTIM upper time bin boundaries, from low to high, defined as the array TIMB(I),I=1,NTIM. The first lower time boundary is always 0.0. The same four methods that are allowed for defining the energy boundaries may also be used to define the time bin boundaries.

- For NTYPE > 0, a record containing NTYPE particle types in any order, defined as the array ITIP(I),I=1,NTYPE. The allowed particle types are listed in Table 2.2. (Since the $\pi^0$is not

transported, it cannot initiate an event; therefore it is not included in the allowed input list at the present time).

- For NPARM > 0, a record containing NPARM cell, material, or surface numbers (integers), as appropriate, in any order, for which one wishes a tally to be made; these are defined as the array LPARM(I),I=1,NPARM. At the present time, for editing a HISTP written by LAHET or a HISTX written by HMCNP, these are the *code* cell and *code* surface identifiers as defined by the MCNP geometry routines, rather than the user names for the same entities. If a null record ("/") is supplied with NPARM > 0, it is treated as "**1,2,3, ... ,NPARM/**". Material numbers are defined by the order in which they appear in the MCNP input. (Note: a different meaning for NPARM is used for IOPT = 13.)

- For NFPRM > 0, a record containing NFPRM upper cosine bin boundaries, defined as the array FPARM(I),I=1,NFPRM. The first lower cosine boundary is always -1.0. If a null record is supplied, equal cosine bin boundaries from -1.0 to 1.0 will be defined by default.

- If NPARM is preceded by a minus sign, a record containing NPARM or NPARM+1 normalization divisors; these are defined in HTAPE as the DNPARM array. The NPARM values are in a one-to-one correspondence with the LPARM array. The last (NPARM+1) entry applies to a total over the NPARM entities where applicable; if omitted, it defaults to 1.0. Through this feature it is possible to input a list of volumes, areas, or masses, as appropriate, obtained from a MCNP calculation. When IOPT > 100, the NPARM cell, surface, or material identifiers are treated as a single entity in constructing a tally edit. In this case, the NPARM normalization divisors are summed to a single divisor. Consequently, one may supply the full list of divisors, if appropriate, or just supply one value for the common tally.

- For IRS > 0, the original source definition record (in LAHET format as described in Section 2.3) followed by the new source definition record (also in LAHET format).

- For ITCONV $\neq$ 0, a LAHET source time distribution record as described in Section 2.3.

- For IRSP $\neq$ 0, three records defining the user-supplied response function:

  ERESP(I),I=1,...,NRESP a monotonically increasing energy grid on which the value of the response function is tabulated;

  FRESP(I),I=1,...,NRESP the values of the response function at the above energies;

  IRESP(I),I=1,...,NRESP-1 interpolation scheme indicators, where IRESP(I) indicates the interpolation scheme to be used for the response function in the I-th energy interval.

  The length NRESP $\leq$ 200 is obtained from the array ERESP input (terminated by a "/"). The user must maintain the proper correspondence among the arrays (see Section 3.6 below).

- Any additional input required for the particular option. For basic option types 1, 2, or 11, this may be the specification of surface segmenting. For basic option types 9, 10, or 12, it is the collimating window definition. Also, for basic option types 1, 9, 11, or 12, an arbitrary vector for angular binning may be input.

The order of the input records as they appear in the INT file is illustrated in Table 3.3.

3.2 HTAPE EDIT OPTIONS

3.2.1 IOPT = 1 or 101 : Surface Current

Option 1 tallies the particle current across the NPARM designated surfaces; it is analogous to the MCNP F1 tally. It uses record types NCOL = 4 and 7 on HISTP and NCOL = 7 on HISTX. If IOPT is preceded by a minus sign, the weight binned is multiplied by the particle energy. The number of energy bins is given by NERG. The number of particle types for which surface crossing data is to be tallied is given by NTYPE and must be > 0. If NPARM = 0, total escape from the system will be tallied when the particle enters an external void; however no contribution will be obtained from a HISTX written by HMCNP, since all records on HISTX are treated as internal boundary crossings (NCOL = 7). When NPARM > 0, current will be tallied on NPARM surfaces; a total over surfaces is not performed. Any of the above particle types may be specified. Binning into NFPRM cosine bins is defined by the value of KOPT. For KOPT = 0 or 5, the cosine is taken with respect to the normal to the surface at the crossing point. For KOPT = 1 or 6, the cosine is taken with respect to the x-axis. For KOPT = 2 or 7, the cosine is taken with respect to the y-axis. For KOPT = 3 or 8, the cosine is taken with respect to the z-axis. For KOPT = 4 or 9, the cosine is taken with respect to an arbitrary vector to be read in.

If KOPT = 5, 6, 7, 8, or 9, the current tallies are binned according to a slicing of each surface into NSEG+1 segments by NSEG planes. In this case, an additional record of the following form is required: "**IFSEG,NSEG,FSEG(1), . . . ,FSEG(NSEG)/**". For IFSEG = 1 the segmenting planes are perpendicular to the x-axis, for IFSEG =2 the y-axis, and for IFSEG = 3 the z-axis. The FSEG(I) are the coordinates of the NSEG planes in increasing order.

For KOPT = 4 or 9, an additional record must be supplied with the direction cosines of the arbitrary vector with which cosine binning is to be made. The form of this record is "**CN(1),CN(2),CN(3)/**", where the parameters input are the direction cosines of the arbitrary vector with respect to the x-, y-, and z-axes. The vector need not be normalized.

The surface current tally represents the time-integrated current integrated over a surface area and an element of solid angle. Unless otherwise normalized, it is the weight of particles crossing a surface within a given bin per source particle. As such, it is a dimensionless quantity.

3.2.2 IOPT = 2 or 102 : Surface Flux

The surface flux tally is analogous to an MCNP F2 tally. It uses record types NCOL = 4 and 7 on HISTP and NCOL = 7 on HISTX. All particle types listed above may be specified. The number of energy bins is given by NERG. The number of particle types for which surface flux data is to be tallied is given by NTYPE and must be > 0. NFPRM is unused. If KOPT = 1, surface segmenting is performed as in option 1 above; the same input record to designate the segmenting planes must be included as in option 1. If IOPT is preceded by a minus sign, the particle weight is multiplied by its energy before tallying.

The surface flux tally represents the time-integrated flux integrated over surface areas. Unless otherwise modified, it is a dimensionless quantity.

3.2.3 IOPT = 3 or 103 : Particle Production Spectra

Option 3 may be used to tally the spectra of particles produced in nuclear interactions. It accesses all collision records (NCOL = 2 or 6) on HISTP for all particles causing collisions. If IOPT is preceded by a minus sign, the edit is performed only for events initiated by the primary (source) particles. For KOPT = 0 or 1, separate edits are performed for cascade and evaporation phase production. In addition,

total nucleon production from either phase is edited. For KOPT = 2 or 3, only the cascade production is edited. For KOPT = 4 or 5, only the evaporation phase production is edited. For KOPT = 6 or 7, only the total nucleon production is edited. For KOPT = 8 or 9, only the pre-fission evaporation production is edited. For KOPT = 10 or 11, only the post-fission evaporation production is edited. If KOPT is even, the edit is over cell numbers; if KOPT is odd, the edit is over material numbers. If NPARM is zero, the edit is over the entire system. The parameters NTYPE and NFPRM are not used. If KPLOT = 1, a plot is made of each edit table. With KOPT = 0 or 1, the cascade production for neutrons and protons is simultaneously plotted (as a dotted line) with the total production.

Unless otherwise modified, tally option 3 (or 103) represents the weight of particles emitted in a given bin per source particle. As such, it is a dimensionless quantity.

3.2.4 IOPT = 4 or 104 : Track Length Estimate for Neutron Flux

Option 4 is analogous to the MCNP F4 tally. It uses the NCOL = 2, 4, 6, and 7 records for neutrons on HISTP only; it uses the NCOL = 5 pseudocollision records if they are present. It applies only to neutrons. If IOPT is preceded by a minus sign, the weight tallied is multiplied by the neutron energy. At the present time, editing is by cell number only and no time binning is allowed. The parameters NTIM, NTYPE, and NFPRM are unused.

Tally option 4 (or 104) represents the time- and volume-integrated particle flux, being a sum of particle weight times track length per source particle. Unless otherwise modified, it has the dimensions of *centimeters*.

3.2.5 IOPT = 5 or 105 : Residual Masses and Average Excitation

Option 5 provides an edit by mass number A of the calculated residual masses and the average excitation energy for each mass. The option accesses the NCOL = 2 and 6 records on HISTP for all interacting particle types. The edit is performed for both the final residual masses and the residuals after the cascade phase. If IOPT is preceded by a minus sign, the edit is performed for events initiated by primary (source) particles only. For KOPT = 0, the edit is by cell numbers; if KOPT = 1, the edit is by material numbers. If NPARM = 0, the edit is over the entire system. The parameters NTIM, NTYPE, and NFPRM are immaterial. KPLOT = 1 will produce plots of each edit table.

Tally option 5 (or 105) represents the particle weight producing a given nuclide per source particle; as such it is a dimensionless quantity. The mean excitation is in units of MeV.

3.2.6 IOPT = 6 or 106 : Energy Deposition

Option 6 provides an edit of energy deposition with a detailed itemization by mechanism. The option requires the NCOL = 2, 3, 4, 6, and 7 records on HISTP as well as the NCOL = 5 records for unstable particles; these are just the records written to HISTP under the default. Since some items may not be locally deposited, user judgement is necessary in interpreting the total energy deposition. If KOPT = 0, binning is by cell number; if KOPT = 1, binning is by material number. A total over the entire system is provided; if NPARM = 0, only the system total will be calculated. Time binning is allowed, but parameters NTYPE, NERG, and NFPRM are unused. Unless otherwise modified, the tally units are MeV per source particle.

3.2.7 IOPT = 7 : Mass and Energy Balance

Option 7 provides an itemized energy balance over processes calculated by LAHET. The option requires the NCOL = 1, 2, 3, 4, 6, and 7 records on HISTP as well as the NCOL = 5 records for unstable

particles; these are just the records written to HISTP under the default. Positive contributions arise from the source and current into a region; negative contributions arise by local deposition, leakage out of a region, and conversion into untransported mass and energy. If KOPT = 0, the edit is by cell number; if KOPT = 1, the edit is by material number. A system total is provided; if NPARM = 0, only the system total is provided. Parameters NTIM, NERG, NTYPE, and NFPRM are unused. Option 7 requires the LAHET data file, BERTIN. Unless otherwise modified, the tally units are MeV per source particle.

The scaling-law procedures used with nucleons above 3.5 MeV and pions above 2.5 MeV do not conserve energy. In addition, there are some remaining features of the low energy calculation that produce relatively small imbalances.

3.2.8 IOPT = 8 or 108 : Detailed Residual Mass Edit

Option 8 provides a detailed edit of residual masses by Z and N, by Z only, by N only, and by mass number A. The option accesses the NCOL = 2 and 6 records on HISTP for all interacting particle types. If IOPT is preceded by a minus sign, the edit is performed only for events initiated by primary (source) particles. If KOPT = 0 or 1, the edit is of the final residual masses. If KOPT = 2 or 3, the edit is of the residuals after the cascade phase and before evaporation. If KOPT = 4 or 5, the edit is of masses immediately preceding fission. If KOPT is even, the edit is by cell number; if KOPT is odd, the edit is by material number. If KPLOT = 1, plots will be produced for each edit table. Parameters NERG, NTIM, NTYPE, and NFPRM are unused. If IXOUT = 1, an auxiliary output file appropriate for input to the ORIHET program will be written. Unless otherwise modified, tally units are dimensionless (particle weight producing a nuclide per source particle).

3.2.9 IOPT = 9 or 109 : Surface Current with Collimating Window

Option 9 is identical to option 1 except that a rectangular or circular "window" is imposed on each surface and the tally made within and without the window. It uses record types NCOL = 4 and 7 on HISTP and NCOL = 7 on HISTX. The window is defined by the intersection of a rectangular or circular tube parallel to the x-,y-, or z-axis with the tally surface. A window definition record appears in place of the segmenting record of option 1. For KOPT = 0, 1, 2, 3, or 4, the window is formed by the rectangular tube; the window record has the following allowed forms:

parallel to x-axis:	1,y(min),y(max),z(min),z(max)/
parallel to y-axis:	2,z(min),z(max),x(min),x(max)/
parallel to z-axis:	3,x(min),x(max),y(min),y(max)/

For KOPT = 5, 6, 7, 8, or 9, the window is formed by a circular tube (cylinder); the window record has the following allowed forms:

parallel to x-axis:	1,y(center),z(center),radius/
parallel to y-axis:	2,z(center),x(center),radius/
parallel to z-axis:	3,x(center),y(center),radius/

3.2.10 IOPT = 10 or 110 : Surface Flux with Collimating Window

Option 10 is identical to option 2 except that the edit is performed inside and outside a "window" defined as in option 9. It uses record types NCOL = 4 and 7 on HISTP and NCOL = 7 on HISTX. Instead of the segmenting record of option 1 a window definition record appears, whose form is described in option 9. For KOPT = 0, the rectangular form is used, and for KOPT = 1, the circular form is used. Parameter NFPRM is unused.

3.2.11 IOPT = 11 or 111 : Pulse Shape of Surface Current

For each defined bin, option 11 provides an edit of the current crossing a surface in an energy and angle bin, the mean time $\bar{t}$ of crossing in the bin, the standard deviation σ of $\bar{t}$ given by $(\overline{t^2} - \bar{t}^2)^{\frac{1}{2}}$, the figure of merit F.O.M. 1 given by (current)/σ^2, and the figure of merit F.O.M. 2 given by (current)/σ^3. It uses record types NCOL = 4 and 7 on HISTP and NCOL = 7 on HISTX.

Unless otherwise modified, the current tally is dimensionless. The units of $\bar{t}$ and σ are nanoseconds, while F.O.M. 1 is in ns^{-2} and F.O.M. 2 is in ns^{-3}. The parameter FNORM is used to adjust the units of the time variable, which are nanoseconds in LAHET, and does *not* modify the surface current edit. Thus to convert from nanoseconds to microseconds, use FNORM = 0.001. The bin definition is identical to option 1, including surface segmenting, except that NTIM is unused.

3.2.12 IOPT = 12 or 112 : Pulse Shape of Surface Current with Window

Option 12 provides the same edits as option 11 with the same bin definition as option 9 using a collimating "window". It uses record types NCOL = 4 and 7 on HISTP and NCOL = 7 on HISTX. The input is identical to option 9, with the exception that NTIM is unused.

3.2.13 IOPT = 13 : Global Emission Spectrum

Option 13 tallies the number of particles per unit solid angle entering the external void region with direction cosine falling within a segment of solid angle; as such, it represents the angular distribution of the emitted particles at a very large distance from the interaction region. The option uses any NCOL = 4 leakage records on HISTP and *all* records on HISTX indiscriminately. Energy binning is specified by the usual methods. The number of energy bins is given by NERG. The number of particle types for which surface crossing data is to be tallied is given by NTYPE and must be > 0. The polar angle bins (representing lines of latitude) are defined by entering the NFPRM cosine values in the FPARM array. Binning in the azimuthal angle ϕ, corresponding to lines of longitude, is determined by the value of NPARM, which defines NPARM equal azimuthal angle bins from a lower bound of 0°on the first bin to an upper bound of 360°on the last bin. The value of KOPT determines the orientation used to define the angles as shown in Figure 3.1. The allowed options are as follows:

KOPT = 1: the +z-axis defines the polar angle and ϕ is measured counter-clockwise from the +x-direction;

KOPT = 2: the +z-axis defines the polar angle and ϕ is measured counter-clockwise from the +y-direction;

KOPT = 3: the +x-axis defines the polar angle and ϕ is measured counter-clockwise from the +y-direction;

KOPT = 4: the +x-axis defines the polar angle and ϕ is measured counter-clockwise from the +z-direction;

KOPT = 5: the +y-axis defines the polar angle and ϕ is measured counter-clockwise from the +z-direction;

KOPT = 6: the +y-axis defines the polar angle and ϕ is measured counter-clockwise from the +x-direction.

A value of KOPT = 0 defaults to KOPT = 1. For NPARM $\geq$ 1, a null record "/" must be supplied in place of the LPARM array; NPARM = 0 defaults to NPARM = 1, but the null record need not be supplied. If a null record is supplied for the FPARM array, NFPRM equal cosine bins from -1.0 to 1.0 are supplied.

Note: surface crossing records appearing on a HISTX are not distinguished as to whether they correspond to an internal surface crossing or to escape into the external void. (On a HISTP, the escape records are designated by NCOL = 4.) For the purposes of option 13, any surface crossing record on HISTX, whether edited separately or in a MERGE edit with HISTP, is treated as leakage into the external void.

The following is an example of the input for using option 13:

```
Title 1: Option 13 Example
Title 2: 100 Equal Solid Angle Bins
13,-10,,1,1,10,10,4*,1/
-0.5,800./
1/
/
/
```

In this case, the energy is binned in 10 equal lethargy intervals of half-decade width below 800 MeV and normalized per MeV. No time binning is done. Only neutrons are edited. The z-axis determines the polar angle and the azimuthal angle is measured from the x-axis. Ten azimuthal angle bins are used and 10 equal polar angle cosine bins are defined by taking the default. The flag IMERGE is non-zero to indicate a merging of HISTP and HISTX to produce a spectrum tabulation for both high and low energy neutrons. Note that the last four records could be written on one line as "**-0.5,800./1///**".

Tally option 13 may be considered as the time-integrated particle current integrated over a sphere in a void at a very large distance for the interaction region. Since it is normalized per unit solid angle, the units are dimensionless, being sr^{-1} per source particle.

3.2.14 IOPT = 14 or 114 : Gas Production

Option 14 provides an edit of hydrogen and helium gas production, by isotope, by element, and total. It accesses all NCOL = 2, 3, and 6 records caused by particles which are isotopes of hydrogen and helium. Unless modified by FNORM, the units of gas production are atoms per source particle. If KOPT = 0, the edit is by cell number; if KOPT = 1, the edit is by material. NERG, NTIM, and NTYPE are unused.

3.3 THE RESOURCE OPTION

The RESOURCE option allows the user to edit the data available on a history file while altering the assumed spatial distribution of the source from that used in the original LAHET/HMCNP calculation. The option is invoked by setting the input flag IRS = ± 1; the two options provide for norming the output edits in different ways, as described below, but use the same underlying principles. The user must insert into the HTAPE input file a record corresponding to the source input record of the original LAHET run followed by a LAHET-type source record describing the source distribution he wishes to apply to the output edits. (See Section 2.3).

The mathematical formulation of the various LAHET source options as probability distributions is shown in Section 2.3. In general, a source point is obtained at a point (x_0', y_0') in a plane by sampling

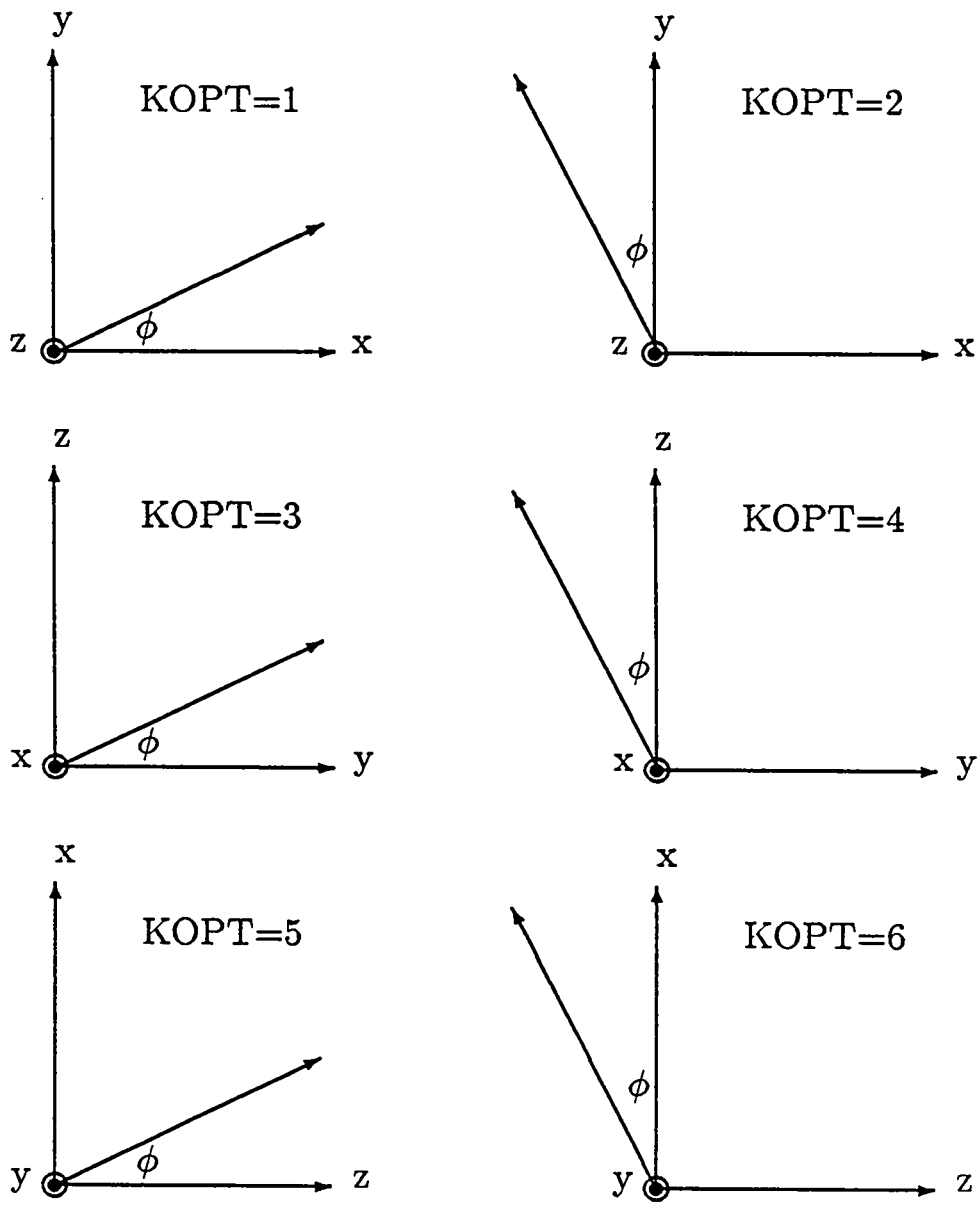

Figure 3.1: Use of the KOPT Parameter for HTAPE Option 13

from a specified distribution $p_0(x'_0, y'_0)$; the laboratory coordinates of the source point (x, y, z) are then obtained for any z by applying a transformation $(x'_0, y'_0) \Rightarrow (x, y)$. Application of the RESOURCE option consists in obtaining estimates from a different probability distribution of the coordinates (x, y) than was used in the LAHET calculation. For any given history i, the source coordinates (x_i, y_i) are obtained from the source record (NCOL = 1); they are, of course, a unique characteristic of the entire history. By using the original source specification, we may obtain the inverse transformation

$$(x_i, y_i) \Rightarrow (x'_{0i}, y'_{0i})$$

and from the new source specification we obtain the inverse transformation

$$(x_i, y_i) \Rightarrow (x'_i, y'_i).$$

Note that a single point in laboratory coordinates may define different values for the coordinates in the spaces used for sampling the original and the new source distributions. A weight factor f_i is then calculated by

$$f_i = p(x'_i, y'_i)/p_0(x'_{0i}, y'_{0i})$$

where $p(x', y')$ is the probability distribution implied by the new source definition and $p_0(x'_0, y'_0)$ is the original probability distribution. If q_i is any quantity that would be tallied from history i without the RESOURCE option, then the modified tally is obtained by the substitution $q_i \Rightarrow f_i q_i$.

The existence of the above mentioned coordinate transformations also implies the existence of the transformation of the probability densities

$$p_0(x'_{0i}, y'_{0i}) \Rightarrow \tilde{p}_0(x_i, y_i)$$

and

$$p(x'_i, y'_i) \Rightarrow \tilde{p}(x_i, y_i)$$

for any source point (x_i, y_i) in laboratory coordinates. If we define

$$f(x, y) \;=\; \tilde{p}(x, y) \;/\; \tilde{p}_0(x, y)$$

we then have

$$f_i \;=\; f(x_i, y_i).$$

Define the set $\mathbf{S_0}$ by

$$(x, y) \in \mathbf{S_0} \quad iff \quad \tilde{p}_0(x, y) \;\neq\; 0$$

and the set $\mathbf{S}$ by

$$(x, y) \in \mathbf{S} \quad iff \quad \tilde{p}(x, y) \;\neq\; 0.$$

Since $\tilde{p}(x, y)$ vanishes outside of $\mathbf{S}$, and since all sampled source points lie in $\mathbf{S_0}$, f_i is non-zero only if (x_i, y_i) is an element of the intersection set $\mathbf{S}' \;=\; \mathbf{S} \bigcap \mathbf{S_0}$. The expectation value of f_i is then given by

$$E(f_i) \;=\; \int_{\mathbf{S}'} f(x, y)\tilde{p}_0(x, y)\; dx\; dy \;=\; \int_{\mathbf{S}'} \tilde{p}(x, y)\; dx\; dy\;.$$

The one additional output quantity from a RESOURCE computation is the sample mean of f_i given by

$$\bar{f} \;=\; \frac{1}{N}\sum_{i=1}^{N} f_i$$

where N is the number of histories in the LAHET run. If $S \subseteq S_0$, then $S' = S$ and $E(\bar{f}) = 1$; otherwise $E(\bar{f}) < 1$. An example of overlapping source regions is shown in Figure 3.2. The original source was sampled from the set of points S_0 lying inside the rectangle. The source implied by the distribution we are imposing with the RESOURCE option would potentially have been sampled from the set of points S lying within the square. For this case, not all of S is included in S_0, so that $E(\bar{f}) < 1$; since not all of S_0 is included in S, some histories will not contribute to the tallies.

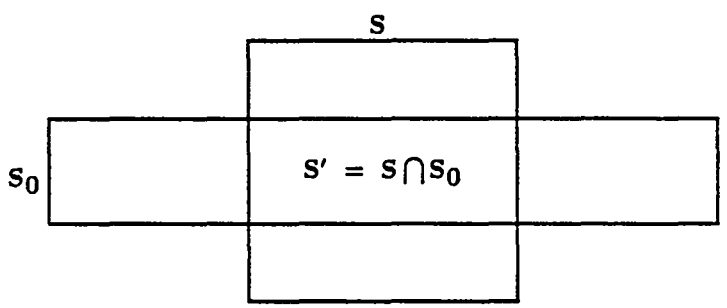

Figure 3.2: Example of Overlapping Source Regions

The two different methods for computing the mean of an estimate obtained by tallying q_i are determined by the sign of the IRS input flag according to the following definitions:

$$\bar{q}_+ = \frac{\sum f_i q_i}{\sum f_i} \quad \text{for IRS} = +1 \ ;$$

$$\bar{q}_- = \frac{\sum f_i q_i}{N} \quad \text{for IRS} = -1 \ .$$

The estimate of $\bar{q}_+$ is a ratio of random variables and the estimation of the error in $\bar{q}_+$ involves the variance of the denominator and the covariance between the numerator and denominator as well as the variance of the numerator; they are combined according to the usual rules of combining errors. The estimation of the error in $\bar{q}_-$ is conventional.

In the case that the new source distribution lies completely within the old ($S \subseteq S_0$), the *expectation values* of $\bar{q}_+$ and $\bar{q}_-$ are the same. $\bar{q}_+$ represents the summed response normed by the weight of the source particles which were *actually* produced in S. It will produce a lower variance than the alternative method, but has the disadvantage of being a ratio of random variables. $\bar{q}_-$ is, in effect, the summed response normed by the *expected* weight of source particles lying within S: $\bar{q}_- = \bar{f}\bar{q}_+$. The variance contains an additional contribution arising from the fluctuation of the weight of particles appearing in S from its expected value.

To illustrate this point, consider the artificial case where the response $q_i = q_0$ is a constant. Then $\bar{q}_+ = q_0$ and is a zero variance estimator. On the other hand, $\bar{q}_- = q_0\bar{f}$ and fluctuates with the weight of sampled points lying within S. However, since in this case S lies *completely* within S_0, we have $E(\bar{f}) = 1.0$ and $E(\bar{q}_-) = q_0$.

When S is *not* a subset of S_0, the interpretation of the norms of $\bar{q}_+$ and $\bar{q}_-$ differs greatly. When the RESOURCE option is not in effect, the basic norm for all tallies is " per source particle ", that is, per particle in the beam defined by the specified probability distribution over the entire set S_0. When IRS = -1, the norm becomes " per source particle " over the set S, i.e., in the entire beam as defined by the new probability distribution. (Of course, that fraction of the weight of the new source lying outside S_0 will contribute 0 to a tally). As the extent of the new source greatly exceeds the extent of the old, or as the overlap goes to zero, $E(\bar{f}) \rightarrow 0$ and $E(\bar{q}_-) \rightarrow 0$. Nonetheless, the interpretation of the norm remains simple since it refers to the *entire beam* defined by the new source. With IRS = +1, when $E(\bar{f}) \rightarrow 0$ the tallied quantity $E(\bar{q}_+)$ approaches a finite limit. It represents the contribution from a source distribution normalized over the set S′, which is always limited in extent by the original source. It may be interpreted as the contribution for a beam whose profile is described by the probability distribution $p(x, y)$ defined only on S′.

Let us apply our artificial example ($q_i = q_0 =$ *constant*) to the overlapped source regions illustrated by Figure 3.2. As before, $\bar{q}_+ = q_0$ and $\bar{q}_- = q_0\bar{f}$. If we make the further assumption that the original and the new source distributions are *uniform* over the areas for which they are defined, we obtain the following results. Let

$$A_{S_0} \equiv \text{area represented by } S_0;$$

$$A_S \equiv \text{area represented by } S;$$

$$A_{S'} \equiv \text{area represented by the intersection } S' .$$

Then

$$\bar{p}(x, y) = \frac{1}{A_S}$$

for (x, y) within S and vanishing otherwise. Similarly,

$$\bar{p}_0(x, y) = \frac{1}{A_{S_0}}$$

for (x, y) within S_0 and vanishing otherwise. As a consequence,

$$f_i = \frac{A_{S_0}}{A_S} \cdot$$

when (x, y) lies in the intersection region S′ and is 0 otherwise. Therefore,

$$E(\bar{f}) = \frac{A_{S_0}}{A_S} \int_{S'} \bar{p}_0(x, y)\, dx\, dy = \frac{1}{A_S} \int_{S'} dx\, dy = \frac{A_{S'}}{A_S}$$

so that

$$\bar{q}_- = \frac{q_0 A_{S'}}{A_S} \quad .$$

We see then that $\bar{q}_+$ estimates the tally as if the problem had been run with a source distributed *only* over the set S′, whereas $\bar{q}_-$ estimates the tally as if the problem had been run with a source distributed over the *entire* square S, with a score coming *only* from those histories whose source coordinates also lie with the rectangular region S_0 of the original source.

The use of IRS = +1 is probably advantageous when all (or nearly all) of the particle weight defined by the new source comes from source points lying within the original source definition. The option IRS = -1 may be valuable when the new source definition overlaps the old significantly. In this case, the difficulty of interpreting the results for IRS = +1 may arise in trying to determine a factor FNORM to change the normalization, when it may be difficult to integrate the given probability density functions over the intersection subset S′.

3.4 THE MERGE OPTION

The objective of the MERGE option is to allow data from a HISTP (written by LAHET) and data from a HISTX (written by HMCNP) to be edited concurrently into a single tally. Neutron surface crossing data may appear on either file; a single energy bin and a total over energy may contain contributions from either source with a proper computation of the estimated standard deviation. Photon surface crossing data will appear only on HISTX, while data for other particles will appear only on HISTP; together with the combined neutron data, all may be edited in the execution of a single case.

Note that only surface crossing records for neutrons and photons are written by HMCNP onto HISTX, according to the specifications described in Chapter 4. At the present time, the TALLYX subroutine used in HMCNP cannot distinguish whether a surface crossing will enter an external void (importance 0) region or enter another internal cell. Consequently, all records on HISTX are identified as internal surface crossing (NCOL = 7) records. This condition will cause an error in executing edit option 13 unless *only* records corresponding to leakage into the external void have been written onto HISTX.

3.5 THE TIME CONVOLUTION OPTION

Assume that an initial LAHET calculation has been made with the default source time distribution (i.e., all histories start at t=0). A time-dependent tally for *any* of the allowed LAHET source time distributions may then be made with HTAPE without rerunning the LAHET calculation. The same LAHET calculation can provide results for a arbitrary number of source time distributions using time convolution.

The method works by dividing the contribution to a tally, which would normally be credited to a unique time and to a single time bin, into contributions to all time bins according to the weighting implied by the specified time probability distribution. With respect to the distribution of initial source time, this is an application of "the method of expected values." As such, it eliminates that contribution to the variance in a time bin that arises from sampling the time variable of the source, and is generally preferable to applying a time distribution in the LAHET run itself.

3.6 THE RESPONSE FUNCTION OPTION

Any non-zero value of the IRSP parameter allows the user to apply an energy-dependent response function $F(E)$, where E is the particle energy, to the current and flux tallies given by edit option types 1, 2, 4, 9, 10, and 13. The user supplies a tabulation of the function $F(E)$ by the pairs of values FRESP(I), ERESP(I) which are input as the arrays ERESP(I),I=1,...,NRESP and FRESP(I),I=1,...,NRESP described in Section 3.1. The element IRESP(I) of the third input array then specifies an interpolation scheme for computing the response function value within the interval ERESP(I) $< E \leq$ ERESP(I+1). For IRSP > 0, the interpolated response function value *multiplies* the tally increment; for IRSP < 0, it *divides* the tally increment.

There are five interpolation schemes that may be specified individually for each energy interval in the response function tabulation, using the following values for IRESP(I).

1. Constant: the response function value is the value at the lower energy of the interval.

2. Linear-linear: the response function is interpolated linearly in energy.

3. Linear-log: the response function is interpolated linearly in the logarithm of the energy.

4. Log-linear: the logarithm of the response function is interpolated linearly in energy.

5. Log-log: the logarithm of the response function is interpolated linearly in the logarithm of the energy.

Any value of IRESP(I) outside the range [1,5] is treated as 1 (i.e., constant over the interval).

The energy range for the specified response function need not span all possible particle energies in the problem. If a particle energy falls below ERESP(1), then FRESP(1) is used as the value of the response function. Similarly, if a particle energy exceeds ERESP(NRESP), then FRESP(NRESP) is used as the value of the response function.

3.7 EXECUTING HTAPE

The LCS version of HTAPE, to which this description applies, is available from the Common File System as **/LCS/HTAPE**. If option 7 is requested, the LAHET data file BERTIN must be in the ⇒ user's file space; HTAPE will read it from the CFS if necessary.

The default file name for the input is INT, the default file name for the output is OUTT, the default file name for a LAHET-written history file is HISTP, and the default file name for the HMCNP-written leakage file is HISTX. These file names may be defined by file replacement, so that the most general execute line is "**HTAPE INT=... OUTT=... HISTP=... HISTX=... / t v**". If both the files HISTP and HISTX are present in the user's file space, and either is to be edited separately, then one or the other must be suppressed by including either HISTP=0 (if HISTX is desired) or HISTX=0 (if HISTP is desired) on the execute line. However they may be edited together using the MERGE option described above in Section 3.3.

If the plotting option is invoked, a CGS metafile PLOT will be produced. Additional option-dependent output files may be generated with the IXOUT option.

3.8 MODIFYING HTAPE

The HTAPE code may usually be easily modified (by a user familiar with the HISTORIAN utility) to obtain a special edit by making a small modification of an existing edit option. To do so, the user may access a number of files on the CFS node "**/LCS**".

The first of these files is COSHTAPE, a COSMOS input file that illustrates how the standard version of HTAPE is updated. The second is HTAPEI, an HISTORIAN input file that contain any recent updates to HTAPE and instructions that suggest how a user might obtain a listing of the code. To prepare a special version of HTAPE, the user should create his own version of the HISTORIAN input file HTAPEI by appending his changes to the existing file. The instructions necessary to compile and load the new HTAPE are then contained in COSHTAPE.

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Chapter 4

THE HMCNP CODE

4.1 INTRODUCTION

HMCNP is a modification to the MCNP code ([13],[14]) which accepts the NEUTP file from LAHET (for neutrons and perhaps protons and deuterons), the GAMTP file from PHT (for photons), or a merged COMTP file as an input source. In addition, a TALLYX subroutine has been included which provides some tallying options which have proved to be of interest to LAHET users and which will, in addition, cause the writing of a surface crossing file which may subsequently be edited by HTAPE. Versions of HMCNP are identified by the version of MCNP from which they are obtained (currently ⇐
3A and 3B).

Although the principal use of HMCNP has been in conjunction with LAHET, the source routine may be used to input any neutron/photon volume source that has been externally generated in NEUTP format (see Appendix D). Since none of the default MCNP sources have been removed, HMCNP may also be used for conventional calculations.

When accepting a NEUTP format file as a source, HMCNP invokes the special subroutine SOURCE, which reads the source file, controls the banking of source particles, and defines the current history (cascade) number during execution. All particles arising from one LAHET cascade are treated as one history in HMCNP for statistical tallying; the number of LAHET cascades is used to norm the edits and is used as the number of degrees of freedom in computing variances.

Previous versions of HMCNP included the capability for writing a surface crossing file (NEUTX) for particles entering an external void region; that file could be used as a NEUTP for a source in an enlarged problem. With the advent of MCNP version 3A, that function may be performed with the "surface source write (SSW)" and "surface source read (SSR)" options [13]. Therefore, the NEUTX option has been deleted from HMCNP. In addition, the capability to bin surface currents with respect to an arbitrary vector has been adopted in MCNP version 3B [14], so that such a function is no longer performed in the TALLYX subroutine of HMCNP. Version 3B includes the capability of transporting protons and deuterons in multigroup mode; LAHET and the NEUTP file format have been modified ⇐
accordingly.

4.2 EXECUTING HMCNP

The latest version of HMCNP is at the level of MCNP version 3B. The executable file is available to users as HMCNP3B or HMCNP under the CFS node "/LCS". The older executable version based on

MCNP version 3A is still available as HMCNP3A under the same CFS node.

To use HMCNP, the user must invoke the SOURCE subroutine by the *absence* of the SDEF, SSR, and KCODE records in the INP input file. In addition, the user must supply a FILES record to define the input source files and any output file. The following is suggested as an example of the usage of the FILES record for accessing a sequence of NEUTP files and generating the optional HISTX file as described above:

FILES 77 NEUTP S U 0 78 NEUTPA S U 0 79 NEUTPB S U 0 70 HISTX S U 0

The user should note that it is necessary to specify on the FILES record all of the continuation files (NEUTPA,NEUTPB,...) of NEUTP generated by LAHET. For a GAMTP created by PHT, or a merged file COMTP created by MRGNTP, *only the first file of a family need be specified;* standard system file family techniques will access the continuations. *Warning:* a maximum of six files may be specified on a FILES record.

If the NPS record is absent, or if NPS is greater than or equal to the number of cascades run in the LAHET problem, HMCNP will process all the source information and norm the output to the total number of cascades. If NPS is *less* than the number of cascades in the source, HMCNP will process all source records up to and including cascade number NPS and norm the output to NPS. If an unexpected end of file is encountered on the source input file, HMCNP will terminate gracefully with the last appearing cascade and norm the output accordingly.

4.3 HMCNP3B TALLYX ROUTINE

For HMCNP3B, the default TALLYX subroutine [13] may be used to write a HISTP-like file of particle surface crossings for tallying with HTAPE; it also provides tallying capabilities similar to those of HTAPE option 9. Either or both of two operations may be performed for F1 type (surface current) tallies. First, a surface crossing record may be written into a HISTP-like file defined as unit 70 (and conventionally known as HISTX); unit 70 must be specified on the FILES record. Second, the current tally may be divided into two user bins representing current inside and outside of a user-specified rectangular or circular window ("collimator") without using surface segmenting. The user must supply an FU record on a type 1 current tally to utilize the TALLYX features, and, for the second option, must supply specifications on an RDUM record. Either one or two parameters are specified on the FU record. The *first* parameter on the FU record controls the writing of the surface crossing file. The allowed values are the following:

> 0	surface record written	tally is performed;
0	surface record written	tally is suppressed;
< 0	no record written	tally is performed.

The latter case may be used to utilize the window definition without any other modifications; it is otherwise unneeded.

Some warnings to the user must be made. First, all records written to HISTX are labeled as "internal boundary crossing" (NCOL = 7) even if they represent "escape from the system" (NCOL = 4); this may cause problems when using HTAPE options IOPT = 1 or IOPT = 13. Second, if FU records which specify writing to HISTX are assigned to two or more type 1 tallies referring to the *same surface*, then crossing records for that surface will be written two or more times; subsequent editing with HTAPE will then erroneously score the same crossing event two or more times.

The name HISTX is suggested for the file created by this option. HISTX is the default file name used by HTAPE for a file so generated. The HISTX file will family by standard system procedures, and will always family on a restart run.

If the window option is desired, the user must supply one of the following values as the *second* parameter on the FU record and the corresponding entries on the RDUM card:

1	the window is	$\mathrm{RDUM}(1) < \mathrm{Y} < \mathrm{RDUM}(2), \mathrm{RDUM}(3) < \mathrm{Z} < \mathrm{RDUM}(4)$;
2	the window is	$\mathrm{RDUM}(1) < \mathrm{Z} < \mathrm{RDUM}(2), \mathrm{RDUM}(3) < \mathrm{X} < \mathrm{RDUM}(4)$;
3	the window is	$\mathrm{RDUM}(1) < \mathrm{X} < \mathrm{RDUM}(2), \mathrm{RDUM}(3) < \mathrm{Y} < \mathrm{RDUM}(4)$;
4	the window is	$(\mathrm{RDUM}(1) - \mathrm{Y})^2 + (\mathrm{RDUM}(2) - \mathrm{Z})^2 < \mathrm{RDUM}(3)^2$;
5	the window is	$(\mathrm{RDUM}(1) - \mathrm{Z})^2 + (\mathrm{RDUM}(2) - \mathrm{X})^2 < \mathrm{RDUM}(3)^2$;
6	the window is	$(\mathrm{RDUM}(1) - \mathrm{X})^2 + (\mathrm{RDUM}(2) - \mathrm{Y})^2 < \mathrm{RDUM}(3)^2$.

4.4 HMCNP3A TALLYX ROUTINE

For the older HMCNP version 3A, the default TALLYX subroutine provides the option that the angular binning may be defined with respect to a coordinate axis or an arbitrary vector rather than the normal to the surface; this feature is a standard option in HMCNP version 3B [14]. The user must supply an FU record on a type 1 current tally to utilize the routine; either one or two parameters are specified on the FU record. The *first* parameter on the FU record controls the writing of the surface crossing file *and* the definition of the cosine used to determine the angular binning. The allowed values are the following:

5	surface record written	surface normal defines the cosine;
4	surface record written	arbitrary vector defines the cosine;
3	surface record written	z-axis defines the cosine;
2	surface record written	y-axis defines the cosine;
1	surface record written	x-axis defines the cosine;
0	surface record written	tally is suppressed;
-1	no record written	x-axis defines the cosine;
-2	no record written	y-axis defines the cosine;
-3	no record written	z-axis defines the cosine;
-4	no record written	arbitrary vector defines the cosine;
-5	no record written	surface normal defines the cosine.

Option -5 may be used to utilize the window definition without any other modifications; it is otherwise unneeded. If options 4 and -4 are used, the user must supply the direction cosines of the arbitrary vector (not necessarily normalized) as the first three entries on an RDUM record. The supplied vector will be used for *all* tallies for which options 4 or -4 are specified.

If the window option is desired the input is specified as above, *unless* options 4 or -4 are used, in which case the window parameters are entered starting with RDUM(4) following the parameters defining the arbitrary vector.

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Chapter 5

THE PHT CODE

5.1 THEORY

The PHT code is used to construct a gamma-ray source file from the collision information recorded on a LAHET history file for use as a source for HMCNP in a mode 1 or 2 problem. PHT may also be used to calculate gamma production cross sections from a LAHET run made with option N1COL = -1. In either case, PHT requires the NCOL = 2 and NCOL = 6 nuclear interaction records on the HISTP file as input.

The gamma ray output of PHT arises from two sources: from the decay of neutral pions and from the deexcitation of residual nuclei. For the decay of neutral pions, only the two-gamma decay mode is allowed. For the deexcitation of the residual nuclei, the assumption is made that all particle decay modes have been exhausted; thus gamma emission does not compete with particle emission.

It is assumed that there exists a range of known energy levels, above which there is a continuum of energy levels with level density given by the Gilbert-Cameron formulae [17]. The library of level data is based on the CDRL82 library, with over 50,000 listed levels. If the excitation energy of a residual nucleus lies between two levels, it is assigned randomly to one or the other of the levels with a probability that depends linearly on the distance from the levels. If the excitation is above the maximum known level, it is assumed the level is in the continuum.

The probability of a transition between levels is assumed to be proportional to the Weisskopf single particle estimates [18] unless specified by the library. For levels in the continuum and for known levels with unknown spin and parity, a spin state is randomly assigned using the Gilbert-Cameron spin densities to generate a sampling distribution; parities, at the present time, are assigned with equal probabilities. For a transition within the continuum to a state of given spin, the transition probability is also proportional to the level density for the final spin state.

The gamma cascade proceeds from the above assumptions. For an excitation energy lying in the continuum, transition to another level in the continuum competes with transitions to known levels. If the initial excitation energy lies within the known levels, or a level has been reached by transition from the the continuum, the probability of a transition to lower levels is obtained from library data if available or from the model otherwise. When specified in the library data, a 0^+ to 0^+ transition is permitted to occur without gamma emission (representing internal conversion).

The user has the option of selecting the level of the physics model to be used in the PHT calculation. It is possible to ignore the experimental branching ratios and perform a pure model calculation. The user may also choose to treat all transitions as E1 transitions, corresponding to the model previously employed by Troubetzkoy [19].

The proper kinematics are used to obtain the energy and angle distribution for the pion decay gammas. However, at the present time, the emission of deexcitation gammas is assumed to be isotropic in the laboratory frame, ignoring nuclear recoil.

5.2 INPUT FOR PHT

The input file for PHT (default name INPH) follows the same pattern as HTAPE input. It has the following structure:

- Two records of title information (no slashes allowed), 80 columns each.
- An option control record (list-directed format).
- Additional input as required by the chosen options (list-directed format).

At the present time, only single-case execution is allowed.

The option control record defines the options to be used and the additional input required. The structure of this record is

ITAPE,ICC,NERG,NPRG,NPARM,NFPRM,FNORM,KPLOT/

The meaning of these parameters is as follows:

1. ITAPE defines the output option; the default is ITAPE=1.
   - For ITAPE = 0, no GAMTP will be written.
   - For ITAPE = 1, GAMTP will be written containing both pion decay gammas and deexcitation gammas.
   - For ITAPE = 2, GAMTP will contain only deexcitation gammas and a second file, GAMTP1, will be written containing the pion decay gammas.
   - For ITAPE < 0, it is assumed that the LAHET run was made with N1COL = -1; no GAMTP is generated.

   For ITAPE $\geq$ 0, the printer and plotter output is the gamma energy spectrum, per cascade. For ITAPE < 0, the printer and plotter output are gamma production cross sections; in this case, the normalization of the output is performed according to the rules applicable to the XSEX code (see Section 6.1).

2. ICC defines the level of physics to be applied. Values of 0 through 4 are allowed. The definitions of the physics options defined by ICC are discussed below. The default is ICC = 4.

3. NERG defines the number of energy bin boundaries to represent the deexcitation gamma spectra. The default is 2000.

4. NPRG defines the number of energy bin boundaries to represent the pion decay gamma spectra. The default is 100.

5. NPARM defines the number of cells over which to tally gamma spectra. Gamma source output is from the entire system, regardless of NPARM, and the spectrum over the system is always generated. NPARM = 0 is the default and only the spectrum over the system is generated. The maximum of NPARM is 400.

6. NFPRM defines the number of cosine bins for representing the pion decay gamma spectrum. It is generally useful only when ITAPE < 0, to produce double-differential cross sections, since the binning is always with respect to the z-axis (the assumed beam direction). The default is NFPRM = 0. The maximum is 400.

7. FNORM is an overall multiplicative normalization factor to be applied to the printer and plotter output. The default is FNORM = 1.0. When using ITAPE < 0 to obtain cross section output, FNORM may be used as described in chapter 6 for the XSEX code.

8. KPLOT is a flag to turn on plotting. A value of 0 implies no plotting and a value of 1 requests plots. The default is 0.

According to the parameters specified on the option control record, the following records are required in the order specified:

- For NERG > 0, a record defining NERG upper energy bin boundaries for editing the deexcitation gamma spectrum is required. The NERG energies may be entered, from low to high. Any of the four methods for entering energies used by HTAPE may be used to input these NERG energies. If a null record (/) is given, a default bin width of 10 keV is used.

- For NPRG > 0, a record defining NPRG upper energy bin boundaries for editing the pion decay gamma spectrum is required. They may be specified as in the preceding paragraph, with the exception that a null record will provide a default bin width of 10 MeV.

- For NPARM > 0, a record must be provided listing the NPARM cell numbers, in any order, for which gamma spectra are desired. At the present time, these are the *code* cell numbers as defined on the LAHET output by the MCNP geometry routines. There is no default.

- For NFPRM > 0, a record must be provided listing the NFPRM upper cosine bin boundaries for editing the pion decay gamma spectrum. The lower limit on the edits is always -1.0. If a null record is present (only a slash), the range (-1,+1) is divided into NFPRM equal intervals.

5.3 THE PHT PHYSICS MODEL OPTIONS

5.3.1 ICC = 0: The Continuum Model

When ICC = 0 is specified, the continuum is assumed to exist at all nuclear excitations above the pairing gap for the residual nucleus. As a consequence, there is no line spectrum but rather only a continuous gamma energy distribution. All transitions, within the continuum or from the continuum to the ground state, are assumed to be E1 transitions.

5.3.2 ICC = 1: The Troubetzkoy (E1) Model

For ICC = 1, the nuclear energy levels specified in the data library are used. The continuum is assumed to begin above the highest specified level. However, all transitions, whether continuum-to-continuum, continuum-to-level, or level-to-level, are assumed to be E1 transitions.

5.3.3 ICC = 2: The Intermediate Model

When ICC = 2, the model employed is really a hybrid between models 1 and 3. The nuclear levels, and their spins and parities, are obtained from the data library. The continuum begins above the highest

specified level. However, all levels above the lowest that has unknown spin or parity are considered to also have unknown spin. All transitions within or from the continuum, or that involve a level with unknown spin, are treated as E1 transitions as in model 1. All transitions involving only states of known spin and parity utilize the Weisskopf single particle transition model as in option 4.

5.3.4 ICC = 3: The Spin-dependent Model

The ICC = 3 option gives the full model as described in section 5.1, with the exception that any experimental branching ratios are ignored and a pure model calculation is performed for the transition probabilities using the Weisskopf single particle transition estimates.

5.3.5 ICC = 4: The Full Model with Experimental Branching Ratios

With ICC = 4, the full procedure described in section 5.1 is employed, including the use of library-specified branching ratios when available.

5.4 EXECUTING PHT

The default file name for PHT input is INPH. The default file name for printed output is OUTPH. The default file name for the input LAHET history file is HISTP. The default file name for the output gamma source is GAMTP; optionally, as described below, a second gamma source file with only pion decay gammas may be produced with the default file name GAMTP1. The default file name for the nuclear data input library file is PHTLIB. These default names may be altered by file replacement on the execute line. In addition, a CGS plotter metafile called PLOT may be generated.

The latest version of PHT may be obtained, along with the data library, by executing

MASS GET DIR=/LCS PHT PHTLIB .

However, if no PHTLIB is present in the user's local file space, the code will access the Common File
⇒ System to fetch the default PHTLIB. The appropriate execute line is then

PHT INPH=... OUTPH=... PHTLIB=... HISTP=... GAMTP=... / t v

or perhaps

PHT INPH=... OUTPH=... PHTLIB=... HISTP=... GAMTP=... GAMTP1=... / t v .

No parameters are needed on the execute line if all default file names are used.

The GAMTP (or GAMTP1) file may be used directly as a source for HMCNP in a mode 2 problem. In addition, GAMTP may be merged with NEUTP using the MRGNTP utility code (see appendix A) to produce a combined source file (COMTP) for a mode 1 execution of HMCNP; in this case, all the gammas arising both from the high energy interactions and from the low energy neutron interactions will be transported (and tallied) together. The PLOT file may be examined with PSCAN or routed to any of the standard plotting devices.

Chapter 6

THE XSEX CODE

6.1 METHOD

XSEX is the code which analyzes a history file produced by LAHET and generates double-differential particle production cross sections for primary beam interactions. Cross section plots may also be generated.

The execution of XSEX assumes that the LAHET run was made using the option N1COL = -1. Under that option, the incident particle interacts directly in the specified material in which the source is located without any transport; the only possible outcomes are a nuclear interaction or no interaction. Since there is no way to avoid the LAHET geometry input, the user should define a region containing the material for which the cross sections are desired and locate the source in that region. To avoid possible error, only one material should be defined.

The definition of the calculated double-differential cross sections computed by XSEX is given by

$$\frac{(number\ of\ particles\ produced) \times (geometric\ cross\ section) \times FNORM}{(number\ of\ cascades) \times (width\ of\ energy\ bin) \times (width\ of\ angle\ bin\ in\ steradians)}$$

where FNORM is an input normalization factor and the geometric cross section is that calculated (and printed out) by LAHET. If the material atom density specified in the LAHET run was 1.0, then the geometric cross section will be in units of barns; a normalization factor FNORM = 1000.0 will then produce the cross sections in units of millibarns per MeV per steradian. However, if a real atom density was input to the LAHET run, the geometric cross section will be in units of inverse centimeters and the output cross sections will be macroscopic rather than microscopic. In this case, using FNORM = 1/(atom density) will restore the output to units of barns.

Energy-integrated, angle-integrated, and integral particle production cross sections are also calculated. In addition, the total non-elastic cross section is calculated as

$$\frac{(number\ of\ interactions) \times (geometric\ cross\ section) \times FNORM}{(number\ of\ cascades)}$$

6.2 INPUT FOR XSEX

The input file for XSEX (default name INXS) has the following structure.

- Two records of title information, 80 columns each.

- An option control record (list-directed format).
- Additional records as required by the chosen options (list-directed format).

Multiple cases may be processed; for each case the above input structure applies. When multiple cases are processed, input quantities default to the preceding case. If the title records of the second and subsequent cases contain "/", the record must begin with a "$".

The option control record has the structure "**NERG,NANG,FNORM,KPLOT/**". The meaning of these parameters is as follows.

1. NERG defines the number of energy bins for which cross sections will be calculated. For NERG > 0, an energy boundary record is required. For NERG = 0, only energy-integrated cross sections will be generated. The default is initially 0.
2. NANG defines the number of cosine bins for which cross sections will be calculated. For NANG > 0, a cosine boundary record is required. For NANG = 0, only angle-integrated cross sections will be generated. The default is initially 0.
3. FNORM is an overall multiplicative normalization factor to be applied to all cross sections; applications of FNORM are described above. The default is initially 1.0.
4. KPLOT is a plot control flag. The default is initially 0. If KPLOT = 0, no plots will be produced. For KPLOT < 0, only energy-integrated and angle-integrated cross sections will be plotted. If KPLOT > 0, double-differential production cross sections will be plotted for each energy and angle bin, and for all particle types (the plot file may be voluminous). The plot type for cross section vs. energy plots is determined by |KPLOT|as shown in Table 6.1. At the present time there is no control over particle type, so production cross sections are generated for all the particle types that exit a collision (i.e., all but muons). In addition, plots (and edits) are produced for nucleon cascade production and nucleon evaporation production separately. A sample plot is shown in Figure 6.1, taken from the sample problem in Appendix F.

|KPLOT|	Cross section	Energy
1	log	log
2	log	linear
3	linear	log
4	linear	linear

Table 6.1: XSEX Plot Options

At most two additional records may be required, depending on the values specified for NERG and NANG.

- For NERG > 0, a record is required to specify the NERG upper energy bin boundaries. Any of the four methods that may be used for HTAPE may also be used for XSEX. The lower boundary of the first energy bin is always 0, although for the purpose of making log-log plots it is taken as 0.3 times the upper boundary of the first bin.
- For NANG > 0, a record is required to define the NANG upper cosine bin boundaries. They should be entered from low to high, with the last upper boundary equal to 1.0; the lower limit of the first bin is always -1.0. If a null record is present (only a "/"), then the range (-1,+1) is divided into NANG equal intervals.

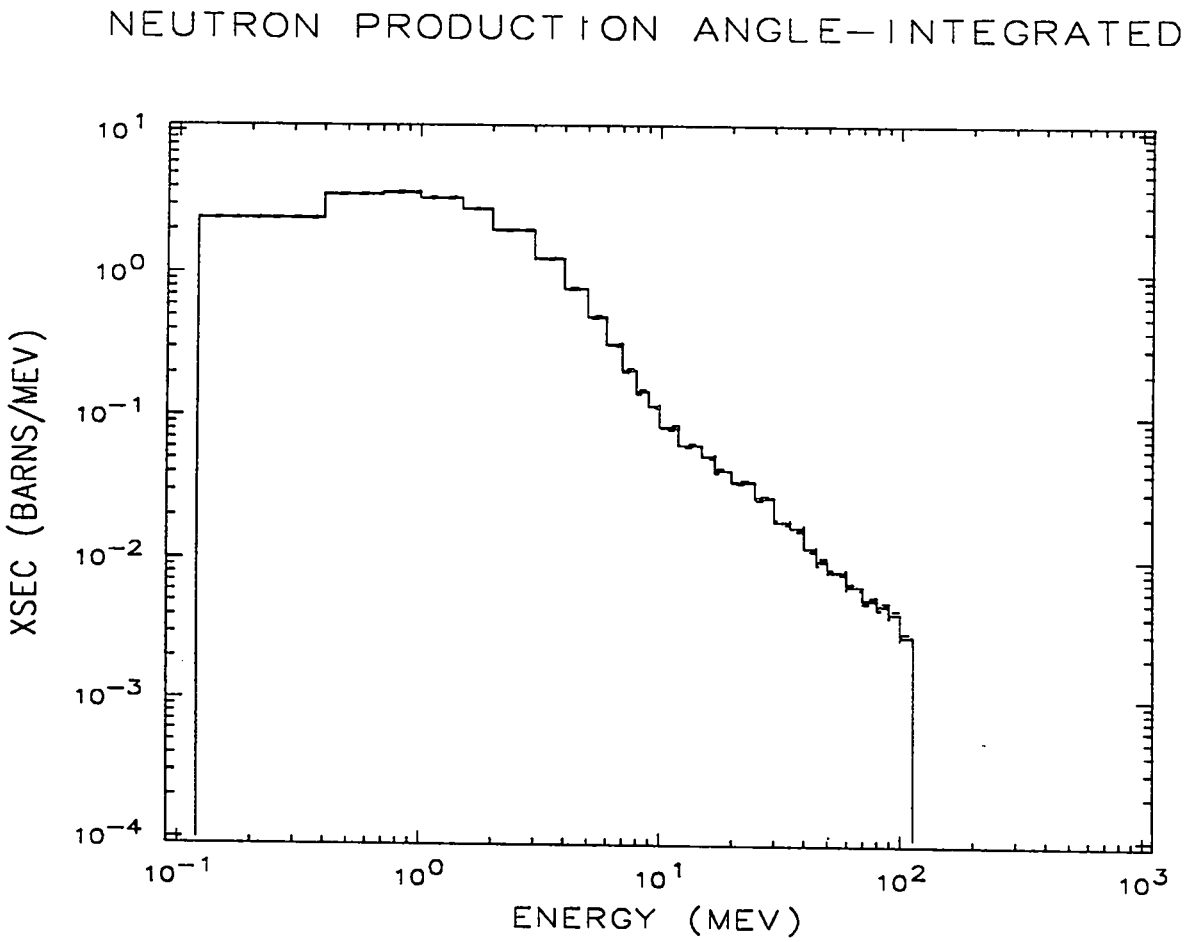

Figure 6.1: Plot Example from XSEX

6.3 EXECUTING XSEX

The executable XSEX file is obtained from CFS by "**MASS GET /LCS/XSEX**". An input file and a history file are the only others required. The default file name for the input is INXS, the default file name for the output is OUTXS, and the default file name for the history file is HISTP. These file names may be changed by file replacement. A PLOT file may also be produced. The appropriate execute line is

XSEX INXS=... OUTXS=... HISTP=... / t v .

The PLOT file is a CGS metafile and may be sent to any of the standard plotting devices. However, one plot is generated for each cross section table and *the number of plots may be very large*; consequently, the user may wish to select individual plots using PSCAN. Each plot that is produced is identified on the OUTXS file, which may be inspected to identify the plots to be output.

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Appendix A

THE MRGNTP CODE

A.1 APPLICATIONS

The utility code MRGNTP is used to merge files in the NEUTP format. It has three major applications:

- When a two-stage LAHET calculation has been made, first in an inner region and then in an outer region, using HISTP from the first problem as the source in the second with the ISRFSR = 1 option, two NEUTP files will have been produced. To obtain a HMCNP calculation which combines both sources of neutrons, it is necessary to merge the two neutron files.

- To obtain the total gamma source in a problem, it is necessary to merge the NEUTP file produced with LAHET with the GAMTP file produced by PHT. The combined file may then be used as a source to HMCNP in a mode 1 problem which treats photons arising both from high energy interactions and from low energy neutron-induced reactions.

- The GAMTP and GAMTP1 files produced by a PHT execution using ITAPE = 2, to obtain separate files of deexcitation gammas and pion decay gammas, may be subsequently merged to obtain combined results from HMCNP.

The LCS version of MRGNTP will merge files in either the new (LAHET) NEUTP format or the old (HETC) NEUTP format, or will merge one file of each format. A description of the old and new NEUTP file formats is given in Appendix D.

A.2 EXECUTING MRGNTP

The MRGNTP utility may be obtained by executing "**MASS GET /LCS/MRGNTP**". No input file is required; all information needed is specified in the execute line. The form of the execute line is "**MRGNTP file-specification / t v**". File specification information need be given only if the user is defining file names by file replacement. The default file names are as follows:

NTP1	the first input file
NTP1A	the first continuation of the first file
NTP1B	the second continuation of the first file
NTP1C	the third continuation of the first file
NTP2	the second input file
NTP2A	the first continuation of the second file
NTP2B	the second continuation of the second file
NTP2C	the third continuation of the second file
NTP3	the output file.

The NEUTP files produced by LAHET do not use system familying routines in generating continuations. Consequently, the names may be changed at will to coincide with the MRGNTP default file names (although only three continuations are allowed). The GAMTP and GAMTP1 files produced by PHT have continuation files created by the system familying methods. For these, only the initial file is referenced by MRGNTP; the continuations are automatically accessed by the code. However, the continuation files in this case must be in the user's local file space with the same name as that with which they were written. Any continuation to the output file NTP3 will be familied by the system.

A.3 EXAMPLE

As an example, let us assume that a LAHET calculation produced a neutron file NEUTP with one continuation file, NEUTPA. The PHT code was then run to produce a gamma source file, GAMTP. It is now desired to combine the neutron and gamma sources for use in a HMCNP mode 1 calculation. Assuming that the files NEUTP, NEUTPA, and GAMTP are in our local file space, and that we wish to give the output file the name COMTP, the appropriate execute line is

```
MRGNTP NTP1=NEUTP NTP1A=NEUTPA NTP2=GAMTP NTP3=COMTP / t v .
```

Appendix B

THE STRIP CODE

B.1 APPLICATIONS

The utility code STRIP is used to extract selected record types from a HISTP file and write a new history file with just the selected record types. Since a LAHET run may produce many long HISTP files, frequent accessing of the files on CFS may be very time consuming. If repeated post-processing is desired, it may be useful to construct an abbreviated history file containing only needed records, thereby saving running time in HTAPE. The following illustrate some possibilities.

- A surface source file, for use with LAHET option ISRFSR = 1, may be created by retaining only type 4 (escape) records.
- A collision file to be input to PHT to generate a gamma source may be created by retaining only type 2 (nuclear interaction) and type 6 (nuclear absorption) records.
- A history file containing only records for a particular particle type may be constructed to permit a HTAPE analysis for just that particle.
- For use with the RESOURCE option in HTAPE, a history file may be created with source (type 1) records as well as other selected records.

B.2 EXECUTING STRIP

The utility code STRIP may be obtained by executing "**MASS GET /LCS/STRIP**". The execute line is then "**STRIP HISTP=... HISTIN=... OUTST=... / t v**". where HISTP is the default file name for the *input* history file and HISTIN is the default file name for the *output* history file. Summary information is written to the printer file OUTST. If no file parameters are specified on the execute line, STRIP will read HISTP and produce HISTIN.

When STRIP is executed, it will prompt the user to enter a list of event types for each allowed particle type. Enter a list of event types, separated by blanks or commas and followed by "/". If all records for a given particle are desired, enter "-1/". If none of the records for a given particle type are desired, just enter "/" or a blank line using the carriage return. The prompts are issued in the following order:

proton ?

neutron ?
pi+ ?
pi- ?

If muons have been transported in the original problem, the following prompts will be issued:

mu+ ?
mu- ?

If ions have been transported in the original problem, the following prompts will be issued next:

deuteron ?
triton ?
He-3 ?
alpha ?

The allowed event types (NCOL values) and their definitions are as follows:

1 source particle record;
2 nuclear interaction;
3 charged particle slowed down;
4 escape (to external void);
5 pseudo-collision;
6 nuclear absorption;
7 internal boundary crossing;
8 multiple scattering event.

STRIP may be run using COSMOS. In the following example of a COSMOS input file, proton source records and neutron leakage records only are written to a file called HISTN4. The pion records are eliminated totally. It is assumed that only nucleons and pions have been transported in the initial calculation, so only four prompts must be answered.

```
*SELECT PRINTLOG=myname
*STRIP HISTIN=HISTN4
1/
4/
/
/
```

Appendix C

HISTP FILE STRUCTURE

C.1 THE EVENT RECORD

The execution of LAHET will produce a binary history file (HISTP) recording the outcome of every particle event. Each such event produces at least one record, the event definition record, of length 38 words. The standard definition of these 38 words is as follows:

1. NCOL: An integer identifying the type of event.

-4	End of run
-3	End of batch
-2	End of file (switch to a new file)
-1	Start of run
0	Not used
1	Source-particle data
2	Nuclear interaction (non-absorption)
3	Charged particle slowed to cutoff
4	Particle escape from the system
5	Pseudo-collision
6	Nuclear absorption[1]
7	Internal boundary crossing
8	Multiple-scattering subtrajectory

2. NOCAS: An integer identifying the current cascade.

3. NAME: An integer identifying the current particle within the cascade.

4. MAT: An integer identifying the medium prior to the current event. For a source particle record (NCOL = 1), the starting random number for the cascade is written in this position.

5. NMED: An integer identifying the medium of the current event. For an internal boundary crossing or an escape, MAT and NMED identify the old and new media, respectively; for all other events, MAT and NMED are the same.

[1] i.e., no particle is emitted during the intranuclear cascade.

6. X: The x-coordinate of the preceding event in centimeters.
7. Y: The y-coordinate of the preceding event in centimeters.
8. Z: The z-coordinate of the preceding event in centimeters.
9. XC: The x-coordinate of the current event in centimeters.
10. YC: The y-coordinate of the current event in centimeters.
11. ZC: The z-coordinate of the current event in centimeters.
12. OLDWT: The statistical weight of the particle before the event at position (XC,YC,ZC).
13. WT: The statistical weight of the particle after the event at position (XC,YC,ZC).
14. E: The kinetic energy of the particle (MeV) at position (X,Y,Z).
15. EC: The kinetic energy of the particle (MeV) at position (XC,YC,ZC).
16. U: The x-direction cosine of the particle at (XC,YC,ZC).
17. V: The y-direction cosine of the particle at (XC,YC,ZC).
18. W: The z-direction cosine of the particle at (XC,YC,ZC).
19. TC: The time variable (nanoseconds) at position (XC,YC,ZC).
20. TIP: The particle type as given in Table 2.2, treated as a floating point number.
21. BOLD: An integer giving the *code* cell number of location (X,Y,Z) as defined by the MCNP geometry routines.
22. BLZ: An integer giving the *code* cell number of location (XC,YC,ZC) as defined by the MCNP geometry routines.
23. LELEM: An integer identifying the number of the surface crossed (for NCOL = 4 or 7), or an integer identifying the nucleus struck within a medium (for NCOL = 2, 5, or 6):

    -1 ^{1}H;
    0 the value given for a pseudo collision;
    I a positive integer identifying the nuclear type, excluding ^{1}H, according to the order in which they are given in the input.

24. NOPART: The number of intranuclear cascade particles produced in a nuclear interaction; for a pseudo-collision, NOPART = -1.
25. NABOV: The total number of intranuclear cascade and evaporation particles produced above their cutoff energies in a nuclear interaction. These are the particles that will be tracked upon leaving the collision.
26. NBELO: The total number of intranuclear cascade particles produced below their cutoff energies in a nuclear interaction.

27. APR: The mass number A of the residual nucleus after both cascade and evaporation (for a non-fission event); APR is set to zero if the residual is one of the emitted particle types. For a fission event, if ATFIS(1) > 0, APR is 1000×ATFIS(1)+ATFIS(2) or, if ATFIS(1) = 0, APR is equal to 1000000+ATFIS(2). For the definition of ATFIS, see Section C.4.

28. ZPR: The charge number Z of the residual nucleus after both cascade and evaporation (for a non-fission event); ZPR is set to zero if the residual is one of the emitted particle types. For a fission event, ZPR is 1000×ZTFIS(1)+ZTFIS(2). For the definition of ZTFIS, see Section C.4.

29. EREC: The kinetic recoil energy of the residual nucleus (MeV) after evaporation for a non-fission event; for a fission event, it is the sum of the recoil energies of both fragments.

30. EX: The excitation energy of the nucleus (MeV) after the cascade phase and before evaporation or fission.

31. HEVSUM: The sum of the kinetic energies of all charged particles, other than protons, which are emitted during evaporation or fission.

32. UU: The excitation energy of the nucleus (MeV) after evaporation for a non-fission event; for a fission event, it is the sum of the excitation energies following evaporation for both fragments.

33. NPART(1): Length of data arrays for evaporation neutrons; for a non-fission event, this is just the number of neutrons evaporated.

34. NPART(2): Length of data arrays for evaporation protons; for a non-fission event, this is just the number of protons evaporated.

35. NPART(3): Length of data arrays for evaporation deuterons; for a non-fission event, this is just the number of deuterons evaporated.

36. NPART(4): Length of data arrays for evaporation tritons; for a non-fission event, this is just the number of tritons evaporated.

37. NPART(5): Length of data arrays for evaporation ^{3}He's; for a non-fission event, this is just the number of ^{3}He's evaporated.

38. NPART(6): Length of data arrays for evaporation alphas; for a non-fission event, this is just the number of alphas evaporated.

For NCOL = 1, EC, XC, YC, and ZC are undefined; the energy and coordinates of the source particle are stored in E, X, Y, and Z. Parameters 27 through 38 are relevant only for NCOL = 2 or 6. Parameters 24 to 26 are relevant only for NCOL = 2, 5, or 6. Parameter 23 is relevant only for NCOL = 2, 4, 5, 6, or 7.

For event records with NCOL < 0, none of the above parameters apply other than NCOL itself. For NCOL = -1 (start of run), the record has the following structure:

NCOL (= -1);
current date (BCD);
time the file was initiated (BCD);
name of the history file (BCD);
current date (again, to distinguish from earlier formats);
the source particle type (integer) from Table 2.2;
thirty-two zero words.

For NCOL = -2 (end of file with continuation to a new file), the record has the following structure:

NCOL (= -2);
name of the current file (BCD);
name of the next continuation file (BCD);
thirty-five zero words.

For NCOL = -4 (end of run), the structure is:

NCOL (= -4);
current date (BCD);
time at end of run (BCD);
total number of NCOL = 1 records;
total number of NCOL = 2 records;
total number of NCOL = 3 records;
total number of NCOL = 4 records;
total number of NCOL = 5 records;
total number of NCOL = 6 records;
total number of NCOL = 7 records;
total number of NCOL = 8 records.
twenty-seven zero words.

For NCOL = -3 (end of batch), only NCOL is written, followed by 37 zero words.

C.2 ABOVE-CUTOFF PARTICLE RECORD

For NCOL = 2, 3, 5, or 6, with NABOV > 0, a record is written which contains the following information for each particle:

NAMEA(I) the internal name of the product particle;

TIPA(I) the type of the product particle from Table 2.2 (floating point);

EA(I) the kinetic energy (MeV) of the product particle;

UA(I) the x-direction cosine of the product particle;

VA(I) the y-direction cosine of the product particle;

WA(I) the z-direction cosine of the product particle;

WTA(I) the statistical weight of the product particle.

The above sequence of information is repeated for each I, I = 1,...,NABOV. For particles arising from evaporation which are above their cutoff energy, the information in this record will duplicate information recorded in the evaporation particle records described below. This record follows the event record when present.

C.3 BELOW-CUTOFF CASCADE PARTICLE RECORD

For NCOL = 2, 3, 5, or 6, with NBELO > 0, a record of the cascade products having kinetic energy below their cutoff is written with the following information:

TIPB(I) the type of the product particle from Table 2.2 (floating point);

EB(I) the kinetic energy (MeV) of the product particle;

UB(I) the x-direction cosine of the product particle;

VB(I) the y-direction cosine of the product particle;

WB(I) the z-direction cosine of the product particle;

WTB(I) the statistical weight of the product particle.

The information is written in the above order for each particle index I, I = 1,...,NBELO. This record follows the " above-cutoff particle record" if present.

C.4 EVAPORATION PARTICLE RECORDS

For each I, I = 1,...,6, with NPART(I) > 0, a record of the evaporation particles of that type is written. The correspondence between the index I and the particle type is as follows:

1	neutrons
2	protons
3	deuterons
4	tritons
5	^{3}He's
6	alphas

The general structure of these six records is:

Statistical weight of the particles.
Energy of 1st particle emitted before fission.
.....
Energy of last particle emitted before fission.
0.0 (if fission has occurred; otherwise, energy data stops).
Energy of 1st particle emitted from 1st fission fragment.
.....
Energy of last particle emitted from 1st fission fragment.
0.0
Energy of 1st particle emitted from 2nd fission fragment.
.....
Energy of last particle emitted from 2nd fission fragment.
X-direction cosine of 1st particle emitted before fission.
Y-direction cosine of 1st particle emitted before fission.
Z-direction cosine of 1st particle emitted before fission.
.....
X-direction cosine of last particle emitted before fission.

Y-direction cosine of last particle emitted before fission.
Z-direction cosine of last particle emitted before fission.
0.0 (if fission has occurred; otherwise, angle data stops).
0.0
0.0
X-direction cosine of 1st particle emitted from 1st fission fragment.
Y-direction cosine of 1st particle emitted from 1st fission fragment.
Z-direction cosine of 1st particle emitted from 1st fission fragment.
.....
X-direction cosine of last particle emitted from 1st fission fragment.
Y-direction cosine of last particle emitted from 1st fission fragment.
Z-direction cosine of last particle emitted from 1st fission fragment.
0.0
0.0
0.0
X-direction cosine of 1st particle emitted from 2nd fission fragment.
Y-direction cosine of 1st particle emitted from 2nd fission fragment.
Z-direction cosine of 1st particle emitted from 2nd fission fragment.
.....
X-direction cosine of last particle emitted from 2nd fission fragment.
Y-direction cosine of last particle emitted from 2nd fission fragment.
Z-direction cosine of last particle emitted from 2nd fission fragment.

In a non-fission event, NPART(I) is just the number of particles of type I which were emitted. In a fission event, NPART(I) is the number of particles of type I that were emitted *plus two*, for all I except I = 4 (tritons). For I = 4, NPART(4) is the number of particles emitted *plus 16*. In this case, the following additional words, describing the fission event, are inserted after the last word of *energy* data:

0.0
Recoil kinetic energy of the 1st fragment.
Initial excitation energy of the 1st fragment.
Total kinetic energy of charged particles other than protons from 1st fragment.
Final excitation energy of the 1st fragment.
Recoil kinetic energy of the 2nd fragment.
Initial excitation energy of the 2nd fragment.
Total kinetic energy of charged particles other than protons from 2nd fragment.
Final excitation energy of the 2nd fragment.
Total kinetic energy of charged particles other than protons before fission.
Final mass number of the 1st fragment ATFIS(1).
Final mass number of the 2nd fragment ATFIS(2).
Final charge number of the 1st fragment ZTFIS(1).
Final charge number of the 2nd fragment ZTFIS(2).

The number of words of angular data in this case is 3×(NPART(4)-14), including the "0.0" words.

C.5 START-OF-RUN RECORDS

For NCOL = -1 (start of run), the event record is followed by six additional records.

1. A 31 word record with the entries:

MAXBCH	(input record 4);
MAXCAS	(input record 4);
MXMAT	(input record 4);
NEUTP	(input record 6);
NPIDK	(input record 6);
N1COL	(input record 6);
NOBALC	(the cascade balance flag obtained from NOBAL on input record 6);
EMIN(I),I=1,...,18	cutoff energies for the 18 particle types;
EMAX	(input record 7);
NEXITE	(input record 6);
NSPRED	(input record 6);
NWSPRD	(input record 5);
NSEUDO	(0 if KREC(5) = 1, 1 otherwise);
LUN	logical unit number used for BERTIN file;
NBERTP	(input record 5);
ICPT	(input record 6);
Five zero words.	

2. The array NEL(M),M=1,MXMAT from input record type 8, giving the number of materials other than ^{1}H in material M.

3. (ZZ(L,M),A(L,M),SIGG(L,M),L=1,NEL(M)): ZZ is the charge number, A is the mass number, and SIGG is the macroscopic geometric cross section for each isotope L in material M.

4. (SIGMX(I,M),I=1,18): the total macroscopic transport cross section for particle type I in material M.

5. (HSIGG(I,M),I=1,18): the maximum macroscopic ^{1}H cross section for particle type I in material M. *Records (3), (4), and (5) are repeated in order for M=1,MXMAT.*

6. (SIGMX(I,MXMAT+1),I=1,18): the total transport cross section in a void for particle type I.

C.6 END-OF-RUN RECORD

After the event record for NCOL = -4 (end of run), a single record is written of the form

((WTSUM(I,J),I=1,18),J=1,8),(NOSUM(I,J),I=1,18),J=1,8)

where WTSUM(I,J) is the total statistical weight of particles of type I generating event records with NCOL = J (including records not written) and NOSUM(I,J) is the actual number of event records with NCOL = J and particle type I written to HISTP.

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Appendix D

NEUTP FILE STRUCTURE

D.1 INTRODUCTION

The NEUTP file consists of a mix of control records and particle records. Each record is 10 words long. Each particle record provides the kinematic parameters for one source particle for HMCNP. The control records have different requirements depending on which option is to be used in HMCNP (see Chapter 4).

The structure of a record is "NN,(SIN(I),I=1,9)". Parameter NN is < 0 for a control record and is > 0 for a particle record, in which case it represents the number of the history with which the source particle is associated. The nine words SIN may be real, integer, or BCD, depending on the record type.

The same file format is used for the NEUTP output by LAHET, the GAMTP file output by PHT, or any merged file output by MRGNTP. Continuation files output by LAHET must be specifically indicated on the FILES card for HMCNP; the end of a file to be continued is indicated by the final record in the file (see NN = -2 below). Files output by PHT or MRGNTP are familied by systems routines; only the first member of the family must be specified on the HMCNP files card.

D.2 CONTROL RECORDS

NN=-1 The first record is always a start-of-run record, with NN = -1. As written by LAHET, or one of its related codes, it has the format "**-1,MAXCAS,MAXBCH,DATE,TIME,0,0,0,0,0**" where MAXCAS and MAXBCH are the number of cascades in a batch and the number of batches in a run as defined in the LAHET input; DATE and TIME are the BCD-coded date and time at which the file was initialized.

NN=-2 The end of one source file and the request for the next continuation file (as written by LAHET) is indicated by a record with NN = -2. The rest of the record is immaterial. The presence of a record with NN = -2 causes the unit number associated with the input source in HMCNP to be incremented by 1 and the next file specified on the FILES card to be accessed.

NN=-3 A record with NN = -3 indicates an end-of-batch as defined by LAHET. The rest of the record is immaterial, and, apart from updating the cascade count, the record has no effect in HMCNP.

NN=-4 A record with NN = -4 indicates an end-of-run condition and is required by HMCNP for all options. Only the value of NN is pertinent.

D.3 PARTICLE RECORDS

For a particle record, all 10 words are meaningful. They have the following definitions in terms of HMCNP variables:

NN a composite NOCAS + ITYP$\times 2^{24}$, where NOCAS is the history (cascade) number of the source
⇒ particle and ITYP is a particle type index given (currently) by 2 for a neutron, 12 for a photon, 1 for a proton, and 8 for a deuteron;

SIN(1) ERG, the particle energy in MeV;

SIN(2) UUU, the x-direction cosine;

SIN(3) VVV, the y-direction cosine;

SIN(4) WWW, the z-direction cosine;

SIN(5) XXX, the x-coordinate;

SIN(6) YYY, the y-coordinate;

SIN(7) ZZZ, the z-coordinate;

SIN(8) WGT, the particle weight;

SIN(9) the time coordinate (in nanoseconds).

In HMCNP, the time coordinate is converted from nanoseconds to shakes with the relationship
⇒ TME = 0.1×SIN(9). The *old format* for NEUTP, accepted by earlier versions of HMCNP, differs from the new in the following items:

NN the history (cascade) number of the source particle;

SIN(1) ±ERG, the particle energy (negative flags a photon).

A positive value of SIN(1) is used to indicated that the particle is a neutron; a negative value indicates a photon. The absolute value of SIN(1) is the energy. However, both HMCNP and MRGNTP will accept either format, or even a mixture of both record types.

Appendix E

ELASTIC SCATTERING DATA

The use of neutron elastic scattering data in LAHET is discussed in Section 2.2. The following data set must be supplied for each element for which neutron elastic scattering data is desired, either on file ELSTIN or within the input file INH. The structure of the data is as follows, modified slightly from [1].

Record type S1 Format (4I5,F10.5,A30)

IDT(1) Element identifier, conventionally $A + 1000Z$ with the mass number A set to 0 for elements with natural isotopic composition (not used internally).

IDT(2) Cross section identifier, conventionally 2 for elastic scattering cross sections (not used internally).

IDT(3) Not used internally.

IDT(4) Number of following records containing elastic scattering cross sections (must be supplied).

FMAS Conventionally, the atomic mass of the element (not used internally).

Thirty characters of information.

Record type S2 Format (2E15.5)
Record type S2 is repeated IDT(4) times, in order of *decreasing* energy.

ES Energy, in MeV, for the elastic scattering cross section.

SIGE Elastic scattering cross section, in barns, at energy ES.

Record type S3 One blank line.

Record type S4 Format (4I5,F10.5,A30)
Same as record type S1, except that IDT(4) refers to the number of records containing $\bar{\mu}$ values and IDT(2) is 71 conventionally.

Record type S5 Format (2E15.5)
Record type S5 is repeated IDT(4) times, in order of *decreasing* energy.

EF Energy, in MeV, for the $\bar{\mu}$ value.

F1 $\bar{\mu}$ value at energy EF.

Record type S6 One blank line.

The following example is the neutron elastic scattering data for ^{12}C taken from file /LCS/ELSTIN.

```
6012    2    0    9            03/16/89  14:09:49
   5.00000e+01    7.10494e-01
   4.50000e+01    7.57178e-01
   4.00000e+01    7.99576e-01
   3.50000e+01    8.33974e-01
   3.00000e+01    8.54964e-01
   2.50000e+01    8.54941e-01
   2.00000e+01    8.24318e-01
   1.50000e+01    7.51146e-01
   1.00000e+01    6.24652e-01

6012   71    0    9            03/16/89  14:09:49
   5.00000e+01    9.27774e-01
   4.50000e+01    9.22029e-01
   4.00000e+01    9.14330e-01
   3.50000e+01    9.03895e-01
   3.00000e+01    8.89438e-01
   2.50000e+01    8.68813e-01
   2.00000e+01    8.38667e-01
   1.50000e+01    7.93480e-01
   1.00000e+01    7.23341e-01
```

Appendix F

SAMPLE INPUT

F.1 THICK TARGET TRANSPORT PROBLEM

F.1.1 The COSMOS Input

The objective of this sample problem is to estimate the neutron, proton, and gamma emission at selected angles from a thick cylindrical target of ^{238}U irradiated by a beam of 256 MeV protons. The COSMOS input file below illustrates all the steps needed to complete the calculation and save the output to the Common File System. Neutron elastic scattering data is supplied through the file /LCS/ELSTIN. The output files NEUTP (from LAHET) and GAMTP (from PHT) are merged into COMTP as a source file for HMCNP3B containing both neutrons and gammas.

```
*select printlog=runlog
*select savel=/088056/samp1/lcs,savef=/088056/samp1/lcs
*mass get wait=on dir=/lcs bertin lahet pht phtlib mrgntp hmcnp3b htape elstin
*mass get wait=on dir=/088056/samp1/lcs inh inp inph int
*lahet
*pht
*mrgntp ntp1=neutp ntp2=gamtp ntp3=comtp
*hmcnp3b
*htape
*switch all. lev. 1
*mass store wait=on dir=/088056/samp1/lcs outh outp outt outph gamtp comtp
*mass store wait=on dir=/088056/samp1/lcs histp histpa neutp neutpa histx
```

F.1.2 The INH File

The geometric description of the problem has the target cylinder extending along the z-axis and enclosed by a 50 cm sphere; the exterior of the sphere defines the extent of the problem. The void within the sphere and exterior to the uranium cylinder is part of the problem; the 0.5 cm radius uniform proton source is located in this void and directed onto the end of the target.

LAHET is executed largely using default options, including the Bertini intranuclear cascade physics. However, the preequilibrium model option IPREQ=1 is selected, and neutron elastic scattering is specified for the uranium (element 23 in the file /LCS/ELSTIN).

```
lahet - 4 cm radius x 5.0 cm thick U238 target - 256 MeV protons -
0.5 cm radius source - 50000 protons

50000,1,1,23,7*,1/
,-1/
/
256./
0,1,1/92,238,.048038,23/
    1  1  -18.98  -1 2 -3
    2  0  -4(1:-2:3)
    3  0  4

    1  cz  4.0
    2  pz  0.0
    3  pz  5.0
    4  so  50.0

in   1 1 0
print

0,256,0.0,-1.0,0.5,0.5,,,0.0,0.0/
```

F.1.3 The INPH File

The PHT execution with the INPH file below specifies that a single GAMTP be written using physics option ICC=4. The gamma production is edited in 20 bins of 1 MeV width for deexcitation gammas and 20 bins of 10 MeV (the default) for pion decay gammas.

```
lahet - 4 cm radius x 5.0 cm thick U238 target - 256 MeV protons -
0.5 cm radius source - 50000 protons
1,4,20,20,0,0,1.0/
1./
/
```

F.1.4 The INP File

For the execution of HMCNP3B, the INP file has the same geometric definition as the INH file. A coupled neutron-photon execution is specified. Surface current tallies are invoked on suface 4 (the sphere) for both neutrons and photons. The default TALLYX subroutine is invoked by the FU records; internal editing is suppressed, but escape records are written to the file HISTX for processing with HTAPE. The source is specified on the FILES record to be the COMTP file.

```
lahet - 4 cm radius x 5.0 cm thick U238 target - 256 MeV protons -
c       0.5 cm radius source - 50000 protons
    1  1  -18.98  -1 2 -3
    2  0  -4(1:-2:3)
    3  0  4

    1  cz  4.0
```

```
    2  pz  0.0
    3  pz  5.0
    4  so  50.0

m1      92238.50c    1.0
print
imp:n  1 1 0
files  77 comtp  s u 0  70 histx s u 0
mode   n p
phys:n 20
f1:n   4
fu1    0
f11:p  4
fu11   0
```

F.1.5 The INT File

The HTAPE run produces the final output in three cases. In the first case, neutron and proton emission is edited on surface 4 in angular bins defined with respect to the beam direction (z-axis). The energy grid is user supplied, and the angular bins are chosen to isolate 30, 60, 120, and 150 degrees. In the second case, photon emission is edited on surface 4 with the same angular bin definition; the energy grid is specified by 100 keV bins from 0 to 20 MeV. The third case calculates particle production (from LAHET only), with the production data edited on the same energy grid as the neutron emission data.

```
lahet - 4 cm radius x 5.0 cm thick U238 target - 256 MeV protons -
0.5 cm radius source - 50000 protons
1,39,0,2,3,1,9,1.0,,,,1/
0.5,1.,2.,3.,4.,5.,6.,7.,8.,9.,10.,12.5,15.,17.5,20.,
25.,30.,35.,40.,45.,50.,60.,70.,80.,90.,100.,110.,120.,
130.,140.,150.,160.,170.,180.,190.,200.,220.,240.,256./
0,1/
4/
-0.9063,-0.8192,-0.5736,-0.4226,0.4617,0.5373,0.8434,0.8870,1.0/
lahet - 4 cm radius x 5.0 cm thick U238 target - 256 MeV protons -
0.5 cm radius source - 50000 protons
1,200,0,1,3,1,9,1.0,,,,1/
0.1/
11/
4/
-0.9063,-0.8192,-0.5736,-0.4226,0.4617,0.5373,0.8434,0.8870,1.0/
lahet - 4 cm radius x 5.0 cm thick U238 target - 256 MeV protons -
0.5 cm radius source - 50000 protons
3,39,0,0,0,0,0,0/
0.5,1.,2.,3.,4.,5.,6.,7.,8.,9.,10.,12.5,15.,17.5,20.,
25.,30.,35.,40.,45.,50.,60.,70.,80.,90.,100.,110.,120.,
130.,140.,150.,160.,170.,180.,190.,200.,220.,240.,256./
```

F.2 CROSS SECTION CALCULATION

F.2.1 The COSMOS Input

The following is an example of a COSMOS input file for a calculation of particle and gamma production cross sections for 113 MeV protons on ^{238}U. All output is stored to the CFS, including a plot file.

```
*select printlog=runlog
*select savel=/088056/samp2/lcs,savef=/088056/samp2/lcs
*mass get wait=on dir=/lcs bertin lahet xsex pht phtlib
*mass get wait=on dir=/088056/samp2/lcs inh inxs inph
*lahet
*xsex
*switch plot xplot
*pht
*switch plot pplot
*mass store wait=on dir=/088056/samp2/lcs outh outxs xplot outph pplot histp histpa
```

F.2.2 The INH File

The cross section option (no transport) is invoked by NCOL=-1 on record 6. A simple geometry is constructed containing the target material (with unit atom density to produce output in barns from XSEX); the source point is located in the material. The ISABEL intranuclear cascade model is invoked (with default settings) as is the preequilibrium model (IPREQ=1).

```
LAHET for xsex - U238 - 113 mev protons
20000 protons ISABEL model LAHET2.1 IPREQ=1

20000,1,1,5*,2,,,1/
/
,,,-1/
113./
0,1/92.,238.,1.0/
    1 1.0 -1
    2 0 1

    1  so  50.0

in   1 0
print

0,113.,0./
```

F.2.3 The INXS File

The particle production cross sections are edited on a user-defined energy grid. The angular bins are chosen to isolate the data at 7.5, 30, 60, and 150 degrees. A short plot file is produced containing only angle integrated cross sections; an example from this case is shown in Figure 6.1.

```
LAHET for xsex - U238 - 113 mev protons
20000 protons ISABEL model LAHET2.1 IPREQ=1
29,9,1.0,-1/
.4,.7,1.,1.5,2.,3.,4.,5.,6.,7.,8.,9.,10.,12.,15.,17.,20.,25.,30.,35.,40.,
45.,50.,60.,70.,80.,90.,100.,113./
-.916,-.816,.45,.55,.816,.916,.9829,.9999,1./
```

F.2.4 The INPH File

The gamma production cross section from nuclear deexcitation is edited with energy bins of 100 keV from 0 to 20 MeV. Since there is no π^0production at this low energy, the π^0tallies are turned off.

```
LAHET for xsex - U238 - 113 mev protons
20000 protons ISABEL model LAHET2.1 IPREQ=1
-1,4,200,0,3*,1/
.1/
```

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