Programming Notes: HISTP File Structure for LAHET^{TM} Version 3 and MCNPX^{TM} LA-UR-01-4007

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Abstract

In the LAHET^{TM} Code System, the results of particle transport and interaction are written by the LAHET3 code to a "history file" for subsequent statistical analysis. In adapting physics packages from LAHET3 for use in MCNPX^{TM} , this method has been included for describing the results of interactions (but not transport) arising from the medium- and high-energy interaction physics. The intent of the present document is to provided a documented description of the format of the HISTP file and a definition of the contents of the file. This will generally be of interest to developers of MCNPX and LAHET and of the related processing codes. It should also assist users who wish to create their own output editors or modify the distributed code.

1 INTRODUCTION

In the LAHET^{TM} Code System, the results of particle transport and interaction are written by the LAHET3[1] code to a "history file" (conventional name HISTP) for subsequent statistical analysis by the HTAPE3 and XSEX3 codes. In adapting physics packages from LAHET3 for use in MCNPX^{TM} [2], this method has been included for describing the results of interactions (but not transport) arising from the medium- and high-energy interaction physics. Of course, it is desirable to have all the output processing and editing in the generating code; however, until that is achieved, off-line processing of the history file must suffice.

The intent of the present document is to provided a documented description of the format of the HISTP file and a definition of the contents of the file. This will generally be of interest to developers of MCNPX and LAHET and of the related processing codes HTAPE3, HTAPE3X[3] and XSEX3. It should also assist users who wish to create their own output editors or modify the distributed code.

As a historical note, the use of the history file (or *tape!*) descends from the original HETC code from ORNL. The original format was maintained for many years[4]. The most significant feature that distinguished the designation[5] "LAHET Version 3" (LAHET3 and the codes HTAPE3 and XSEX3) was a new but incompatible format for the HISTP file that was more complete and more informative in the record of nuclear interactions. However, the reader will note that some ancient and irrelevant material is still included in the file initialization records!

The present document may be considered an addendum to the research note[1].

2 THE EVENT RECORD

2.1 The Event Record Type NCOL

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 29 words. Each recordable event is identified by a value of the variable NCOL, with NCOL > 0 identifying an actual event in the simulation process and NCOL < 0 identifying an operational event in producing the HISTP file. The definition of the possible record types is shown in Table 1. *Note: record types NCOL = 1, 4, 7 and 8 are not used in MCNPX.*

2.2 General Form for NCOL > 0

The 29 words in the event record for NCOL > 0 are listed in Table 2 For NCOL > 0, the standard definitions of these variables are as follows.

NCOL	Record Definition
-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 (no particle is emitted during the intranuclear cascade)
7	Internal boundary crossing
8	Multiple-scattering subtrajectory

Table 1: HISTP Record Types

NCOL: An integer identifying the type of event.

NOCAS: An integer identifying the current history.

NAME: An integer identifying the current particle within the history; NAME = 1 for a source particle. *NAME = 1 always in MCNPX.*

MAT: An integer identifying the medium prior to a boundary crossing.

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.

IR0(1), IR0(2): First and second parts of the random number seed starting the history.

IBOLD: An integer giving the *code* cell number of location (X,Y,Z) as defined by the MCNP geometry routines.

IBLZ: An integer giving the *code* cell number of location (XC,YC,ZC) as defined by the MCNP geometry routines. For an internal boundary crossing or an escape, IBOLD and IBLZ identify the old and new media, respectively; for all other events, IBOLD and IBLZ are the same.

TIP: The particle type as given in Table 3, treated as a floating point number.

1	NCOL=1	NCOL=2 or 6	NCOL=3	NCOL=4 or 7	NCOL=5	NCOL=8
2	NOCAS	NOCAS	NOCAS	NOCAS	NOCAS	NOCAS
3	NAME	NAME	NAME	NAME	NAME	NAME
4	IR0(1)	MAT=NMED	MAT=NMED	MAT	MAT=NMED	MAT=NMED
5	NMED	NMED	NMED	NMED	NMED	NMED
6	IR0(2)	IBOLD=IBLZ	IBOLD=IBLZ	IBOLD	IBOLD=IBLZ	IBOLD=IBLZ
7	IBLZ	IBLZ	IBLZ	IBLZ	IBLZ	IBLZ
8	TIP	TIP	TIP	TIP	TIP	TIP
9	X	X	X	X	X	X
10	Y	Y	Y	Y	Y	Y
11	Z	Z	Z	Z	Z	Z
12	undefined	XC	XC	XC	XC	XC
13	undefined	YC	YC	YC	YC	YC
14	undefined	ZC	ZC	ZC	ZC	ZC
15	OLDWT=WT	OLDWT	OLDWT	OLDWT	OLDWT	OLDWT
16	WT	WT	WT	WT	WT	WT
17	E	E	E	E	E	E
18	undefined	EC	EC	EC	EC	EC
19	U	U	U	U	U	U
20	V	V	V	V	V	V
21	W	W	W	W	W	W
22	TC	TC	TC	TC	TC	TC
23	0 or JAJ	LELEM	undefined	JAJ	LELEM=0	undefined
24	undefined	NOPART	undefined	undefined	NOPART=-1	undefined
25	NABOV=0	NABOV	NABOV	NABOV=0	NABOV	NABOV=0
26	NBELO=0	NBELO	NBELO	NBELO=0	NBELO	NBELO=0
27	MNUC=0	MNUC	MNUC=0	MNUC=0	MNUC=0	MNUC=0
28	undefined	EX	undefined	XMU	undefined	undefined
29	undefined	GEOMXS	undefined	undefined	undefined	undefined

Table 2: Event Record Variables for NCOL > 0

X: The x-coordinate of the preceding event in centimeters.

Y: The y-coordinate of the preceding event in centimeters.

Z: The z-coordinate of the preceding event in centimeters.

XC: The x-coordinate of the current event in centimeters.

YC: The y-coordinate of the current event in centimeters.

ZC: The z-coordinate of the current event in centimeters.

OLDWT: The statistical weight of the particle before the event at position (XC,YC,ZC).

WT: The statistical weight of the particle after the event at position (XC,YC,ZC).

E: The kinetic energy of the particle (MeV) at position (X,Y,Z).

EC: The kinetic energy of the particle (MeV) at position (XC,YC,ZC).

U: The x-direction cosine of the particle at (XC,YC,ZC).

V: The y-direction cosine of the particle at (XC,YC,ZC).

W: The z-direction cosine of the particle at (XC,YC,ZC).

TC: The time variable (nanoseconds) at position (XC,YC,ZC).

LELEM: An integer identifying the nucleus struck within a medium [(for NCOL = 2, 5, or 6) as shown below:]

-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.

JAJ: Surface number identifying the surface crossed (for NCOL = 4 or 7) or the surface on which a surface-source particle is started (for NCOL = 1).

NOPART: The number of intranuclear cascade particles produced in a nuclear interaction; for a pseudo-collision or a stopped particle that decays, NOPART = -1.

NABOV: The total number of cascade and evaporation particles or decay particles produced above their cutoff energies. These are the particles that will be tracked upon leaving the collision.

NBELO: The total number of cascade and evaporation particles or decay particles produced below their cutoff energies in a nuclear interaction.

MNUC: The total number of residual nuclei ($A > 4$) after a nuclear interaction; NCOL = 2 or 6 only.

EX: The excitation energy of the nucleus (MeV) after the cascade phase and before evaporation or fission; NCOL = 2 or 6 only.

GEOMXS: Microscopic cross section (barns) appropriate to normalization of cross section calculations in XSEX3; NCOL = 2 or 6 only.

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.	$\overline{p}$
18	17.	$\overline{n}$
19	18.	electron
20	19.	positron
21	20.	neutrino
22	21.	antineutrino

Table 3: Particle Type Identification

XMU: Cosine of the angle between a particle's direction vector and the normal to a surface crossed; NCOL = 4 or 7 only.

The event record for NCOL > 0 may be followed *in order* by these records.

1. For NCOL = 2 or 6 and MNUC > 0, one *residual nucleus record* written for each of the MNUC residual nuclei.
2. For NCOL = 2, 3, 5, or 6 and NABOV > 0, one *above-cutoff particle record.*
3. For NCOL = 2, 3, 5, or 6 and NBELO > 0, one *below-cutoff particle record.*

2.3 Special Forms for NCOL < 0

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 (CHARACTER*8);
  time the file was initiated (CHARACTER*8);
  name of the history file (CHARACTER*8);
  name of code writing the file (CHARACTER*8);
  the source particle index (integer) from Table 3;
  19 zero words (REAL=REAL*4) or 23 zero words (REAL=REAL*8).

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

  NCOL (= -2);
  name of the new continuation file (CHARACTER*8);
  26 zero words (REAL=REAL*4) or 27 zero words (REAL=REAL*8).

- For NCOL = -3 (end of batch), only NCOL is written, followed by 28 zero words.

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

  NCOL (= -4);
  current date (CHARACTER*8);
  time at end of run (CHARACTER*8);
  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;
  15 zero words (REAL=REAL*4) or 17 zero words (REAL=REAL*8).
  1 zero word (LAHET3) or actual number of histories completed (MCNPX)

3 RESIDUAL NUCLEUS RECORD

For NCOL = 2 or 6 and MNUC > 0, the event record is followed by one record of eight words written for each of the MNUC residual nuclei.

APR: The mass number A of the residual nucleus after both cascade and evaporation; APR is set to zero if the residual is one of the emitted particle types.

ZPR: The charge number Z of the residual nucleus after both cascade and evaporation ; ZPR is set to zero if the residual is one of the emitted particle types.

EREC: The kinetic recoil energy of the residual nucleus (MeV) after evaporation.

UU: The excitation energy of the nucleus (MeV) after evaporation.

ECV: The internal conversion energy from the nucleus (MeV) during deexcitation.

UR: The x-direction cosine of the residual nucleus.

VR: The y-direction cosine of the residual nucleus.

WR: The z-direction cosine of the residual nucleus.

4 ABOVE-CUTOFF PARTICLE RECORD

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

NAMEA(I): The internal name of the emitted particle.

TIPA(I) a packed floating point word equal to 100×CLASS+TYPE, where TYPE is the floating point type of the particle from Table 3 and CLASS is the origin code for the particle from Table 4.

EA(I): The kinetic energy (MeV) of the emitted particle.

UA(I): The x-direction cosine of the emitted particle.

VA(I): The y-direction cosine of the emitted particle.

WA(I): The z-direction cosine of the emitted particle.

WTA(I): The statistical weight of the emitted particle.

TCA(I) The emission tine of the emitted particle.

The above sequence of information is repeated for each I, I = 1,...,NABOV. This record follows the "residual nucleus records", if any.

Class	Particle Origin
0.	intranuclear cascade
1.	particle decay
2.	preequilibrium emission
5.	evaporation and deexcitation before fission
6.	evaporation and deexcitation from first fission fragment
7.	evaporation and deexcitation from second fission fragment

Table 4: Particle Origin Identification

5 BELOW-CUTOFF CASCADE PARTICLE RECORD

For NCOL = 2, 3, 5, or 6, with NBELO > 0, a *single record* for the emitted particles having kinetic energy below their cutoff is written with the following information.

TIPB(I) A packed floating point word equal to 100×CLASS+TYPE defined analogously to TIPA(I) above for the below cutoff particles.

EB(I): The kinetic energy (MeV) of the emitted particle.

UB(I): The x-direction cosine of the emitted particle.

VB(I): The y-direction cosine of the emitted particle.

WB(I): The z-direction cosine of the emitted particle.

WTB(I): The statistical weight of the emitted particle.

TCB(I): The emission tine of the emitted 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 any.

6 START-OF-RUN RECORDS

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

1. A 43 word record with the entries:

	Variable name	LAHET3 definition	HTAPE use	MCNPX def.
1	MAXBCH	INH record 4	yes	= 1
2	MAXCAS	INH record 4	yes	assigned
3	MXMAT	INH record 4	yes	assigned
4	LNEUTP	INH record 5 'NEUTP'	no	= 1
5	NPIDK	INH LCA record	yes	LCA record
6	N1COL	INH record 6	yes	assigned
7	NOBALC	INH LEA record	yes	LEA record
8-29	EMIN(I),I=1,...,22	INH EMIN record	yes	assigned
30	EMAX	INH record 7	no	= 3.495MeV
31	NEXITE	INH LCA record	no	LCA record
32	NSPRED	INH LSC record	no	= 1
33	NSTRAG	INH LSC record	no	= 1
34	NSEUDO	0 if KREC(5) = 1, 1 otherwise	no	undefined
35	NBERTP	unit for BERTIN file	no	defined
36	IBERTP	INH record 5 'NBERTP' or 'NBERT'	yes	assigned
37	ICPT	nonzero if ions are transported	no	assigned
38	IPHT	INH LEA record	yes	LEA record
39-43	Five zero words			

The inclusion of some of these items, such as NBERTP, no longer has any conceivable function and may be eliminated or replaced in future releases.

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. Note that SIGG is actually used in LAHET3 only when the new cross section definition procedure is *not* applied; the values are derived from the original LAHET transport cross section method (MODEXS $\neq$ 0). However, SIGG is used indirectly in HTAPE3 to reconstruct isotopic atom fractions in each problem material.

4. (SIGMX(I,M),I=1,22): the total macroscopic transport cross section for particle type I in material M. The SIGMX array is purely archaic and has no present function in LAHET3 or MCNPX, and it is not currently used in HTAPE3 or XSEX3. The values assigned are derived from the original LAHET transport cross section method (MODEXS $\neq$ 0).

5. (HSIGG(I,M),I=1,22): the maximum macroscopic ^{1}H cross section for particle type I in material M. The HSIGG retains meaning in LAHET even for the new cross section definition procedure, but it has no current use in HTAPE3 or XSEX3. *Records (3), (4), and (5) are repeated in order for M=1,MXMAT.*

6. (SIGMX(I,MXMAT+1),I=1,22): the total transport cross section in a void for particle type I. This feature is not currently used; it was originally included in the format to allow the use of an arbitrary δ-scatter cross section, permitting collision estimation of flux in a void!

7 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=1,22),J=1,8),(NOSUM(I,J),I=1,22),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.

References

[1] R. E. Prael, "Release Notes for LAHET Code System with LAHET^{TM} Version 3.16," X-Division Research Note X-5:RN (U) 01-29, LA-UR-01-1655, Los Alamos National Laboratory (June 2001).
http://www-xdiv.lanl.gov/XCI/PEOPLE/rep/

[2] H. G. Hughes, R. E. Prael, and R. C. Little, "MCNPX – The LAHET/MCNP Code Merger," X-Division Research Note XTM-RN(U)97-012, LA-UR-97-4891, Los Alamos National Laboratory (April 1997).
http://www-xdiv.lanl.gov/XTM/hughes/LA_UR_97_4891/cover.html

[3] R. E. Prael, "HTAPE3X for Use with MCNPX", LA-UR-99-1992, Los Alamos National Laboratory (April 1999).
http://www-xdiv.lanl.gov/XCI/PEOPLE/rep/

[4] Richard E. Prael and Henry Lichtenstein, "User Guide to LCS: The LAHET Code System", LA-UR-89-3014, Los Alamos National Laboratory (September 1989).
http://www-xdiv.lanl.gov/XCI/PROJECTS/LCS/lahet-doc.html

[5] Richard E. Prael,"Release of LAHET^{TM} Version 3.0", X-Division Research Note XCI–RN 98–10 (U), LA-UR-00-2116, Los Alamos National Laboratory (January 1998).
http://www-xdiv.lanl.gov/XCI/PEOPLE/rep/