THE HETC/LHI/SGS RADIATION TRANSPORT CODE SYSTEM

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ABSTRACT

In this tutorial paper we discuss the High Energy Transport (HETC)/Light Heavy Ion (LHI)/Spallation Gamma Source (SGS) Monte Carlo radiation transport computer code system, used to transport nucleons, pions, muons, photons, and "light heavy" nuclei with $2 \leq A \leq 10$ through complex materials and geometries. In particular, we present for the first time in a single place a comprehensive, introductory discussion of HETC/LHI/SGS code physics.

I. INTRODUCTION

The nature of the interaction of a high energy particle beam with a complex target is a topic of high recent interest. The main computational tool that currently exists for performing high energy radiation transport through such targets is the HETC/LHI/SGS computer code system. Unfortunately, the existing relevant literature is not well-suited for those seeking a concise, comprehensive, introductory treatment of the subject from a single source. This tutorial paper aims to fill this existing gap in the area of HETC/LHI/SGS code system physics (but does not address code system operation).

The High Energy Transport Code (HETC)/Light Heavy Ion (LHI)/Spallation Gamma Source (SGS) radiation transport code system is a three-dimensional, Monte Carlo, general combinatorial geometry code system used to transport neutrons, protons, pions, muons, photons, deuterons, tritons, He³'s, alpha particles, and other "light heavy" nuclei (so-called ions) with $5 \leq A \leq 10$ through complex materials and geometries (i.e., through possibly thick targets), the allowed kinetic energy ranges being fractions of an electron volt (eV) to tens of GeV for neutrons; a few keV to 14 MeV for photons; several MeV to tens of GeV for protons, pions, and muons; and several MeV per nucleon to 1 GeV per nucleon for LHI's.

The term "system" is used here because HETC/LHI/SGS is really a collection of three and one-half separate codes linked together: (1) HET, which transports high-energy neutrons (≥ 15 MeV)*, protons, pions, and muons; (2) SGS, which calculates the energies of the gamma-ray photons emitted in the

final de-excitation of the excited residual nucleus remaining after a nonelastic* nucleon-nucleus or pion-nucleus collision in HET (note SGS is not itself a transport code); (3) MORSE, which transports low energy neutrons (< 15 MeV)** and does all photon transport; and (3½) LHI, an addition to HET to allow the partial transport (see subsection III.1 for elaboration) of high energy "light heavy" projectiles with $2 \leq A \leq 10$. (Also, as a matter of terminology, the combination of HET and MORSE is referred to as HETC; and HETC [respectively, HET] extended by LHI is referred to as HETC/LHI [respectively, HET/LHI].) Of these three and one-half codes, the three dimensional Monte Carlo MORSE code is the most well-known and has been used widely for many years for "low energy" neutron and gamma radiation transport. Therefore, the MORSE code is not discussed further. (For a discussion of MORSE, see Refs. 1 and 2.)

Although HET is not as well-known as MORSE, it and its predecessors NTC (Ref. 3) and NMTC (Ref. 4) (now both obsolete) have nevertheless been used and updated since the early 1960's. Before 1973, essentially all work on the code was done at Oak Ridge National Laboratory (ORNL); since then, however, when a version of HETC was put into the Radiation Shielding Information Center, improvements and updates have been made at other institutions, primarily Science Applications, Incorporated (SAI) and Rutherford Laboratory, in addition to those continuing to be made at ORNL. (See Ref. 5 for a synopsis of code evolution up until 1979.) It should be pointed out, however, that, despite these improvements and updates, the high energy physics modeling in HET is founded upon the state of knowledge existing in the early 1970's.

The SGS and LHI codes are recent additions to the code system made at SAI by T. Armstrong and collaborators, LHI in its first iteration having been developed in the 1978-81 time frame (based on a model for alpha-particle projectiles discussed in 1971 by Gabriel, Santoro, and Alsmiller [Ref. 6]), and SGS in its first iteration having been developed in the 1979 time frame (based on a model discussed in 1965 by Hill and Simpson [Ref. 7] and refined in 1969 by Shima and Alsmiller [Ref. 8]). The physical modeling in these latter two codes (or, code and one-half) is still being developed, awaiting additions to the currently sparse experimental data (on thick targets) available for use in validation comparisons.

The code system is organized as shown in Fig. 1. The sequence of physics events associated with this organization is briefly as follows. A high energy particle is "born" at the source (source

*This energy boundary may be fixed anywhere between approximately 15 MeV and 20 MeV, depending upon the user's option. The important point is that this energy boundary be the same for HET and MORSE (being the low energy cutoff for the former and the high energy cutoff for the latter). For the purpose of discussion, 15 MeV was arbitrarily selected for this value.

*By a nonelastic collision we mean either (1) a collision in which there is no particle production and the target nucleus has internally absorbed some of the projectile energy, or (2) a collision in which there is particle production.

**See previous footnote.

Figure 1. HETC/LHI/SGS code system organization.

subroutine), traverses the physical system (input geometry and materials) undergoing various nuclear and atomic interactions (HET/LHI), and then--along with any other particles to whose creation it may have led--is terminated relative to HET/LHI through system escape or other physical processes. Neutrons so terminated because of reaching the low energy cutoff limit (an artificial "death" due to code structure [see subsection II.1] rather than any real physical process) are transferred to MORSE, and residual nuclei information is transferred to SGS for gamma-ray production; this gamma production information is subsequently transferred to MORSE. The low energy neutrons then continue, and the photons then begin, their traversal through the physical system until terminated relative to MORSE.

It is our intention in the sequel to discuss the physics involved at each stage of the calculation. We will not discuss code system operation; this information may be found in Refs. 4 and 9-11. Nor will we discuss comparisons with experiment; such comparisons are readily available in most of the references cited herein. In particular, see Ref. 5 for a compilation of papers which present comparisons of calculations and experiments in various technical areas (e.g., space radiations, radiobiology, dosimetry, and accelerator shielding).

The plan of this paper is as follows. The second section treats the HET code. In the first subsection, the source particles are discussed. Then, because particles other than allowed source particles are considered in the code, nonsource particles (so-called "other particles") are discussed in the following subsection. Next, discussed in some detail, are the nuclear and atomic interactions that

the code modeling allows particles to undergo. (Readers who prefer more detail are referred to the referenced literature. This paper is only introductory.) Finally, the last subsection discusses particle termination, i.e., how the particles "die" in the code.

The LHI "half-code" is treated in the third section. As for HET, the source particles and "other particles" are discussed first. Then, in the next subsection, the LHI model (i.e., the model of the light heavy ion itself) and the LHI nuclear and atomic interaction models are discussed. Finally, the LHI section ends with a subsection on particle terminations.

In the fourth section, the SGS code is treated. Since this code deals only with one particle type, photons, and since photons are transported only by MORSE, the only discussion needed here concerns the details of the gamma-ray production model.

Finally, the fifth section presents some observations on possible improvements to the code system.

Note that when the source consists only of protons and/or neutrons with kinetic energies $\lesssim 350$ MeV (roughly the pion production threshold for nucleons on nuclei), then pions and muons are not present in any of the physical processes occurring in the problem. Hence, the reader whose problems involve only such sources will not be concerned with information pertaining only to these latter particles.

II. HIGH-ENERGY TRANSPORT (HET)

This section treats HET code physics. General references are 5, 9, and 12-14. Additional references, giving more detail in specific areas, are given in the appropriate subsections. Note that some statements in this section covering deuterons, tritons, He^3 's and alphas apply only to HET and not to HET/LHI. Precisely how the statements concerned need to be modified in order to hold true for the latter code is the subject of Section III.

1. THE SOURCE PARTICLES.

The source particle types allowed are neutrons, protons, positive and negative pions and positive and negative muons. (Neutral pions are allowed as source particles in principle, but physically "die" essentially the instant they are born, so the code does not bother to transport them.) The initial position and direction of any given source particle are arbitrarily specifiable. The allowed kinetic energies are given in Table 1.

TABLE 1.
ALLOWED KINETIC ENERGIES FOR SOURCE PARTICLES IN HET

Particle Type	Low Energy Cutoff		High Energy Cutoff	
	E_λ (MeV)		E_h (GeV)	
	Adequate	Best	Best (E_C)	Adequate
n	15	50	3.5	100 ^a
p	15 (nuc) 21 (at)	50 (nuc) 1 (at)	3.5	100 ^a
$\pi^\pm$	$\max(1, 0.147 E_\lambda^p)$		2.5	100 ^a
$\mu^\pm$	$\max(1, 0.113 E_\lambda^p)$		$\geq E_h^\pi + 0.033$	

^aThe high energy cutoff is actually indefinite, based upon both physics and programming considerations. HETC has been used successfully for source particles with $E_h \lesssim 1000$ GeV (Ref. 9, p. 2 ff.).

Explanations of the energy ranges indicated in Table 1 are in order at this point. For neutrons, the lower limit comes from considering the energy range of validity of the nucleon/pion-on-nucleus nonelastic collision model used in the code (the so called intranuclear-cascade/evaporation [INCE] model discussed in subsection II.3.a) which, theoretically, should be valid down to approximately 50 MeV, but which, in fact, has yielded reasonable agreement with experiment down to roughly 15 MeV; the 15 MeV limit is routinely used (Ref. 13). For protons, there are two lower limits: one for nuclear interactions, which comes from the same considerations as above for neutrons; and one for atomic interactions, which comes from the fact that, below this energy limit, the range of charged particles in most materials is extremely short compared to the nuclear mean free path. For both nucleons, the "best" upper limit comes again from limitations of the INCE model, which accounts for only single and double pion production in nonelastic nucleon-on-nucleus collisions; and above 3.5 GeV, this limitation on multiple pion production is not physically valid. A very approximate extrapolation model for such collisions above 3.5 GeV extends the upper limit to nominally 100 GeV, although this is not firm (see footnote to Table 1). In any case, the higher the energy, the worse the scaling approximations.

For charged pions, the lower limit, E_{λ}^{π} , is based only upon atomic interactions and is equal to the greater of the two quantities: (1) 1 MeV, and (2) the atomic collision lower limit for protons, E_{λ}^p , multiplied by m_{π}/m_p , where m_{π} and m_p are the pion and proton rest masses, respectively. (For example, if $E_{\lambda}^p = 15$ MeV then $E_{\lambda}^{\pi} = 2.2$ MeV.) The circumstance in (2) arises because the atomic collision slowing-down model in HET (subsection II.3.c) uses, for each medium, one and the same range-vs-energy table for all charged particles to calculate range from energy and energy from range. The ability to use only one table stems from the scaling relation (Ref. 13)

$$R^{\pi}(E_0, E_f) = (m_{\pi}/m_p) R^p((m_p/m_{\pi})E_0, (m_p/m_{\pi})E_f),$$

where $R(\alpha, \beta)$ denotes the distance ("range") traveled by a particle whose energy is degraded from α to $\beta < \alpha$ because of atomic collisions. So if one wants to know about pions whose final energy is E_f^{π} , one only needs to know about protons whose final energy is $E_f^p = (m_p/m_{\pi})E_f^{\pi} > E_f^{\pi}$; i.e., $E_f^{\pi} = (m_{\pi}/m_p)E_f^p$.

In other words, if one knows about protons whose final energy is E , then one knows about pions whose final energy is $(m_{\pi}/m_p)E$.

The "best" upper limit once again comes from the limitations of the INCE model, which allows only single pion production in nonelastic pion-on-nucleus collisions; and above 2.5 GeV this is not a valid approximation. Again the extrapolation model extends the upper limit to nominally 100 GeV.

For muons, the lower limit is based upon atomic interactions: $E_{\lambda}^{\mu} = (m_{\mu}/m_p) E_{\lambda}^p$ (if $E_{\lambda}^p = 15$ MeV then $E_{\lambda}^{\mu} = 1.7$ MeV). There is no upper limit restriction but E_{λ}^{μ} should at least $E_h^{\pi} + (m_{\pi} - m_{\mu})c^2 = E_h^{\pi} + 33$ MeV.

2. OTHER PARTICLES.

In addition to the allowed source particles mentioned above, several other particle types are considered in HET, all of them being direct or indirect

products of nuclear reactions; however, these are not further transported. This is in marked contrast to the source particle types, which (in addition to being producible at the source) are also allowed to be produced in nuclear reactions, but are then further transported. The "other particles" are low energy neutrons ($E \leq 15$ MeV), neutral pions, deuterons, tritons, He^3 's, alphas, and residual nuclei ($A \geq 5$). The treatment of these abandoned particles by HET is discussed in subsection II.4 on particle terminations.

3. PARTICLE INTERACTIONS.

This subsection discusses the interactions in which the various particles may engage. These interactions divide naturally into three categories: nuclear collisions, particle decays and captures, and atomic collisions. In addition to the general references given at the beginning of Section II, specific references for the atomic aspects are 14 and 15 and for the nuclear aspects are 16-19.

a. Nuclear Collisions. Nucleons and charged pions are the only particles allowed to undergo collisions with nuclei of the media in HET modeling. (That is, neutral pions, deuterons, tritons, He^3 's and alphas are not so allowed.) These collisions may be either elastic or nonelastic in principle, although in HET not all possibilities are in fact allowed.

The struck nuclei allowed are those with $A = 1$ or $A \geq 5$ (i.e., deuterium, tritium, He^3 and He^4 are not allowed as media materials) and it is convenient to discuss these two situations, $A = 1$ and $A \geq 5$, separately. In addition, the HET treatment for each of these two situations depends upon whether the incident nucleon/pion has kinetic energy less than or greater than E_C of Table 1 (3.5 GeV for nucleons and 2.5 GeV for pions). The necessity for these divisions based upon A and E is a direct result of the INCE model used by HET to describe nonelastic collisions, but which is inapplicable for $E > E_C$ and $A < 5$.

In summary, then, the discussion of nuclear collisions is divided into four cases:

$$A = 1, E_{\lambda} < E < E_C;$$

$$A = 1, E_C < E < E_h;$$

$$A \geq 5, E_{\lambda} < E < E_C;$$

$$A \geq 5, E_C < E < E_h.$$

and

(For protons, E_{λ} is to be read as the nuclear low energy cutoff.)*

(1) Collision Model.

(a) $A = 1$. In this situation, the struck nucleon is in fact a proton, and experimental free-free nucleon-on-proton and pion-on-proton elastic and inelastic total and differential cross sections are used directly. (Of course, fits to these data are made to infer cross sections at nonexperimental points, and assumptions are made to infer cross sections from theory in regions where there are no experimental data. For detailed discussions of these issues, start with Refs. 12 and 19.)

1. $E_{\lambda} < E < E_C$. For nucleon-proton collisions, elastic scattering and single and double pion production are taken into

*For $E < E_{\lambda}$, particles cease to undergo nuclear interactions: pions are terminated forever, neutrons are terminated relative to HET, and protons continue to undergo atomic interactions until their energy reaches E_{λ}^p whereupon they, too, are terminated forever (see subsection II.4).

account*, while for pion-proton collisions, elastic scattering, single pion production and charge-exchange** are considered.

Since for nucleon-nucleon inelastic collisions, one accounts only for single and double pion production, and since the threshold for production of more than two pions in such collisions is roughly 3.5 GeV, the modeling discussed in the previous paragraph is valid only for incident nucleons with kinetic energy less than 3.5 GeV. Similarly, since for pion-nucleon inelastic collisions, one accounts only for single pion production, and since the threshold for production of multiple pions in such collisions is roughly 2.5 GeV, the modeling discussed in the previous paragraph is valid only for incident pions with kinetic energy less than 2.5 GeV.

2. $E_C < E < E_H$. To treat collisions with hydrogen nuclei of incident nucleons and pions having energies greater than E_C , additional modeling, valid in such an energy regime, must be introduced. HET uses parametric fits to experimental differential cross section data for elastic collisions, while inelastic collisions are treated using both experimental data for total inelastic nucleon-on-proton and pion-on-proton cross sections and analytic fits to other experimental data as input to a calculational method that takes into account multiple pion production (> 2 for incident nucleons and > 1 for incident pions).

(b) $A \geq 5$

1. $E_\lambda < E < E_C$. For this energy range, HET uses the intranuclear-cascade/evaporation (INCE) model to treat nonelastic collisions of nucleons and pions with nuclei. Elastic collisions with nuclei, considered as single entities, are neglected except for those collisions involving incident neutrons with energies ranging from E_λ^n to at most 100 MeV, this upper limit depending upon the cross section data base available for the nuclide involved. (See Ref. 4 for a sample of a suitable cross section compilation.)

The INCE model for nonelastic collisions is based upon the premise that, at sufficiently high energies (a few tens of MeV), the interaction of a nucleon or pion incident upon a complex nucleus can be treated as the interaction of the incident nucleon/pion with the individual nucleons of the nucleus. This premise holds because the de Broglie wavelength of the incident particle is comparable to or smaller than the average distance between the nucleons within the nucleus.

A nonelastic collision is modeled to take place in two successive stages (Fig. 2). In the first stage--the intranuclear cascade--the incident nucleon/pion initially interacts with a single nucleon inside the target nucleus, oblivious to the presence of the other nucleons inside that nucleus,*** creating collision products (p, n, $\pi^\pm$, π^0). For nucleon-nucleon collisions, elastic scattering and single and double pion production are taken into account; and for pion-nucleon collisions, elastic scattering, single pion production, and

Figure 2. Intranuclear-Cascade/Evaporation (INCE) model with gamma emission.

charge-exchange are considered. Note that the cross sections involved here are precisely those used in the $A = 1$ case, augmented to include the possibility that the struck nucleon is a neutron. These collision products (except for π^0 , which is not further transported) may subsequently undergo further collisions with other single nucleons inside the nucleus, giving rise to an intranuclear cascade. The outputs of this stage are: (1) nucleons and pions leaving the nucleus and proceeding on their way (with position, direction, and kinetic energy specified), possibly to collide with nucleons inside other nuclei and thus initiate an internuclear cascade involving many other nuclei; and (2) the residual excited nucleus.

In the second stage--evaporation--the excited residual nucleus remaining at the end of the intranuclear cascade is assumed to have its residual excitation energy equipartitioned among the remaining nucleons, whereupon it decays by "evaporation" of (i.e., isotropic emission of) low energy (≤ 10 MeV), low mass ($n, p, A \leq 4$) particles until emission is no longer energetically feasible (which, for code purposes, means that residual nucleon excitation energy is ≤ 7 MeV), whereupon evaporation then ceases. It should be pointed out that the possibility of fission during this stage is taken into account in the version of HET discussed here, using an extension by Rutherford Labs to take into account fission-evaporation competition; see Refs. 20 and 21. The outputs of this stage are the evaporation/fission particles and the residual nucleus (with residual excitation energy, E^*), none of which are further transported.

It is now assumed that further de-excitation would take place solely by gamma emission, and that this mechanism (i.e., dissipation of E^*) is the only source of gammas in the entire INCE modeling process. However, INCE modeling does not take the further step of proceeding with this emission process. Indeed, in HET, the residual excitation energy, E^* , associated with the potential photons is not actually converted into photons for further transport; rather, E^* is just recorded. This is where the SGS extension to HET comes into play: it takes E^* and converts it to a photon source usable for input to MORSE which then performs the subsequent photon transport. SGS is discussed in Section IV.

*Examples: $p + p \rightarrow p + n + \pi^+$; $p + p \rightarrow p + p + \pi^0$; $p + n \rightarrow p + n + \pi^0$; $p + n \rightarrow p + p + \pi^-$; $p + p \rightarrow p + p + \pi^+ + \pi^-$; $p + n \rightarrow p + n + \pi^+ + \pi^-$.

**Examples: $\pi^- + p \rightarrow \pi^0 + n$; $\pi^+ + n \rightarrow \pi^0 + p$.

***This is not precisely true: the Pauli Exclusion Principle, which excludes those collisions in which the collision products would be in already-occupied states, is taken into account in cascade modeling.

2. $E_C < E < E_h$. As in the case of $A = 1$, the upper limit on multiple pion production allowed in the INCE model requires that additional modeling be introduced in the present situation ($A \geq 5$) as well to account for collisions involving incident particles with $E > E_C$. Briefly, the method used here is to apply scaling relations for energy, angle, and particle multiplicity to extrapolate to higher incident particle energies the results obtained from INCE for nucleons having kinetic energy of 3.5 GeV and pions having kinetic energy of 2.5 GeV. This extrapolation is constrained to be consistent with the sparse experimental data available. Further details are in Ref. 12.

(2) Nuclear Model. In order to describe the interaction of a nucleon or pion incident upon a nucleon within a nucleus to the level of detail required for particle transport, one must specify spatial, momentum, and potential energy distributions for these nuclear nucleons. HET assigns these distributions as follows (Ref. 22).

The nucleon spatial density distribution inside the nucleus is represented as a three-region step-function of radius, corresponding to a central sphere and two surrounding spherical annuli, with the magnitudes of the constant neutron and proton densities in each region chosen to approximate Hofstadter's continuous distribution (Ref. 23). The region boundaries are the same for neutrons and protons, with the neutron-to-proton ratios in each region being the same as that ratio for the nucleus as a whole. The outer radii $r_1 < r_2 < r_3$ of the three regions are those radii at which the monotonically decreasing continuous distribution assumes 90 percent, 20 percent, and 10 percent respectively of its $r = 0$ value.

The nucleon momentum distribution inside the nucleus is assumed to be a zero-temperature Fermi momentum distribution in each region, i ; i.e., $f_{ij}(p) = c_{ij} p^2$ ($j = 1, 2$ distinguishing between neutrons and protons respectively) with constants c_{i1} (resp. c_{i2}) determined such that

$$\int_0^{p_{i1}^F} f_{i1}(p) dp$$

is the total number of neutrons (resp. protons) in region i and p_{i1}^F (resp. p_{i2}^F) is the momentum of a

neutron (resp. proton) corresponding to the Fermi energy. Note that this energy is dependent upon the nucleon density and therefore different for each nucleon type (j) in each region (i). Consequently, the composite momentum distribution for the entire three-region nucleus is not a zero-temperature Fermi distribution but only "piecewise Fermi."

The nucleon potential energy inside the nucleus is taken to be a constant V_{ij} in each region, the value of the constant V_{i1} (resp. V_{i2}) being the sum of the zero-temperature Fermi energy of the neutrons (resp. protons) in region i plus the binding energy of the most loosely bound nucleon, this binding energy being taken to be constant at 7 MeV for all regions and all nuclei.

b. Decays and Captures. HET modeling takes into account pion and muon decay and capture of negative pions by nuclei. (For more detail, see subsection II.4 on particle terminations.)

A positive (negative) pion may decay in flight or at rest (i.e., when its energy falls below E_π) to a positive (negative) muon plus a neutrino (which is ignored). The details of the decay are computed by using the known charged pion lifetime (2.6×10^{-8} s)

and by assuming an isotropic distribution of resulting muons in the pion rest frame. The muon is subsequently transported.

In addition to decaying as just described, a negative pion coming to rest may be captured by a nucleus; the result of such a capture is computed using the INCE model. (In addition to the cross sections mentioned in subsection II.3.a as being taken into account in INCE, π^- absorption cross sections are also included in that model.)

A neutral pion is considered to decay at the place where it is born (since its mean lifetime is approximately 9×10^{-17} s) to two photons. The details of the decay are computed; however, the photons are not actually created and hence are not subsequently transported.

A positive (negative) muon may decay in flight or at rest (i.e., when its energy falls below E_μ) to a positron (electron) plus a neutrino-antineutrino pair (which is ignored). The details of the decay are computed using the known muon lifetime (2.2×10^{-6} s); however, the positrons (electrons) are not actually created and hence are not subsequently transported.

c. Atomic Collisions. Energy loss by protons, charged pions, and muons due to excitation and ionization collisions with the atomic electrons of the material media, and scattering of these transported charged particles by multiple scattering centers, are both taken into account in HET modeling. Consideration of these processes serves to modify the trajectory and energy of a transported particle between two successive nuclear collisions, causing an otherwise straight trajectory to be curved and causing the energy at the end of the trajectory to be lower than that at its beginning.

The basic methodology used to compute energy loss for protons is in essence as follows (Ref. 21). First, for each medium, the standard Bethe-Bloch continuous slowing down approximation is used to compute the proton stopping power, $S(E)$, of the medium as a function of proton energy. Next, the mean proton range for a proton of energy E is computed according to

$$\bar{R}(E) = \int_0^E dE' / S(E').$$

In this way, a [mean] range-vs-energy table is constructed for each medium. To determine the energy loss ΔE of a proton starting with energy E_0 and traveling a distance D in the medium, the energy E_f corresponding to range $R(E_0) - D = R(E_f)$ is determined from the range-vs-energy table for the medium and then $\Delta E = E_f - E_0$ (≤ 0).

To take into account the effect of range straggling, the procedure in the last paragraph is implemented using not the mean range, but the "straggled range," which for a given energy, E , is sampled from the Gaussian density

$$f_E(R) = [1/(2\pi)^{1/2}] \sigma(E) e^{-[\bar{R}-R(E)]^2/2\sigma^2(E)},$$

with variance $\sigma^2(E)$ which may be readily computed (as per Ref. 21).

For charged pions and muons, energy loss is derived from the proton calculations using scaling relations (see the discussion near the end of subsection II.1 of this paper, and Ref. 14).

Multiple coulomb scattering of protons, charged pions, and muons is treated using Fermi's joint distribution function for angular and lateral spread of the scattered particle to correct Rutherford's standard single scattering center cross-section formula for the effect of multiple scattering centers (Ref. 12).

4. PARTICLE TERMINATIONS.

In this subsection we discuss how all the particles considered by HET have their histories terminated. Some of this information was presented previously (see, in particular, the discussion of decays and captures), but it is all presented here systematically. In reading this subsection, reference to Fig. 1 may be useful as an aid in tracking particle bookkeeping issues.

Note that, in addition to the termination modes discussed below, all transported particles (neutrons, protons, charged pions and muons) may also terminate by escape from the system geometry.

A neutron with $E \geq E_{\lambda}^n$ is terminated when its kinetic energy falls below E_{λ}^n (see Table 1), at which time its position, direction and kinetic energy are recorded on the low energy neutron source file for later input to MORSE. Such a record is also made for a neutron born during evaporation with kinetic energy $< E_{\lambda}^n$.

A proton is terminated when its kinetic energy falls below E_{λ}^p , at which time its position, direction and kinetic energy are recorded on the event history file.

A positive pion is terminated by decaying in flight or at rest (i.e., when its energy falls below $E_{\lambda}^{\pi^+}$) to a positive muon (which is subsequently followed) and a neutrino (which is ignored) using the known π^+ mean lifetime.

A negative pion is terminated by decaying in flight to a negative muon (followed) and a neutrino (ignored) using the known π^- mean lifetime. However, in contrast to positive pions, it may be terminated at rest (i.e., when its energy falls below $E_{\lambda}^{\pi^-}$) in one of two possible ways: (1) by decaying to a negative muon and a neutrino (as in flight), and (2) by being captured by a nucleus (and initiating a chain of events treated by the INCE model). Which of these two possibilities actually occurs depends in fact upon the atomic density of the material in which the pion stops; in practice, the user is allowed (and must) specify one of two options: that either every π^- coming to rest anywhere in the geometry will experience a mode 1 termination, or every π^- coming to rest will experience a mode 2 termination.

A neutral pion is terminated at the instant it is born; its position, direction and kinetic energy are recorded on the event history file for possible later use in defining a high-energy gamma-ray source according to $\pi^0 \rightarrow \gamma + \gamma$. (The gammas are not actually created by HET.)

A positive or negative muon is terminated by decaying in flight or at rest (i.e., when its energy falls below E_{λ}^{μ}) to a positive or negative electron (which is not actually created by HET) respectively, plus a neutrino-antineutrino pair (ignored), using the known muon mean lifetime; position, direction, and kinetic energy of the muon are recorded on the event history file for possible later use in defining an electron-positron (and subsequently a high-energy gamma-ray) source. (For example, this information, along with the neutral pion gamma information, could be used as the source for a separate electromagnetic cascade code.)

Deuterons, tritons, He^3 's and alphas are terminated at birth (during the evaporation phase of a nuclear nonelastic collision) in the sense that they are not transported away from the collision site; position, direction and kinetic energy at birth are recorded on the event history file.

Residual nuclei are terminated in exactly the same way as the particles of the preceding paragraph, except that A, Z and residual excitation energy E^*

are also recorded on the event history file in addition to position, direction and recoil kinetic energy. Further (in HET/SGS), A, Z, E^* , and position are also recorded on the residual nucleus file for later input to SGS.

III. HIGH ENERGY TRANSPORT/LIGHT HEAVY IONS (HET/LHI)

This section treats HET/LHI code physics.

General references are 6,15,24 and 25. Additional references, giving more detail in specific areas, are given in the appropriate subsections.

In essence, all HET/LHI does is allow light heavy ions with $2 \leq A \leq 10$ to behave as source particles (in a restricted sense to be discussed later) in what is otherwise just the HET code. Everything that follows in this section is an elaboration of this fact.

1. THE SOURCE PARTICLES AND OTHER PARTICLES

a. Source Particles. HET/LHI extends the source particle types allowed to include not only those source particles allowed in HET but, in addition, deuterons, tritons, He^3 's, alpha particles and other light heavy nuclei with $5 \leq A \leq 10$. (Recall that the first four of these are not allowed as source particles in HET, but only as "other particles.") Again, the initial position and direction of [the center of mass of] any given source particle are arbitrarily specifiable. The allowed kinetic energies for those source particles unique to HET/LHI are given in Table 2; of course, Table 1 also applies to HET/LHI.

TABLE 2.
ALLOWED KINETIC ENERGIES FOR ADDITIONAL SOURCE PARTICLES IN HET/LHI

Particle Type	Binding Energy (MeV)	Low Energy Cutoff (Nuclear)		High Energy Cutoff
		E_{λ} (MeV)		E_H (GeV)
		Adequate	Best	Adequate
d	2.2 ^a	32.2	102.2	~ 2
t	8.5 ^a	53.5	158.5	~ 3
He^3	7.7 ^a	52.7	157.7	~ 3
α	28.3 ^a	88.3	228.3	~ 4
Li^7	39.2 ^b	144.2	389.2	~ 7

^aReference 24.

^bReference 25.

As was the case for protons, there are two low energy cutoffs for each LHI—one for nuclear interactions and one for atomic interactions. The atomic cutoff is simply $E_{\lambda}^I = A \cdot E_{\lambda}^p$, where E_{λ}^p is the proton low energy cutoff for atomic interactions (see Table 1).

The nuclear interaction lower limits in Table 2 are derived from those of Table 1 by requiring that the kinetic energy per nucleon be either 15 or 50 MeV for the adequate or best case, respectively. However, the upper limits in Table 2 do not follow from those of Table 1, but rather from other considerations associated with LHI particle interaction modeling (see subsection III.2.b). These upper limits amount to roughly 1 GeV/nucleon, and even the adequacy of this number has uncertainty to it (Ref. 24, p. 162) since enough experiments have not been done to substantiate the theory; hence, we give only one upper limit, rather than both an "adequate" and a "best" upper limit.

It is important to point out that the multi-nucleon particles mentioned above are elevated only partially to source particle status in HET/LHI (i.e., they are transported); they do not have full source particle status in the sense of HET. That is, an LHI is transported intact only from the source to the site of its first nuclear collision, but not thereafter. After this collision, the individual nucleons of the LHI continue to be transported individually as in HET but are not correlated with each other, in contrast to the situation that existed before the collision. For example, after the very first nuclear collision in its history of, say, an alpha particle, the alpha particle loses its identity, i.e., ceases to exist as an alpha particle, and is not further transported as an alpha particle. Just after the collision, alpha particles may be emitted from the nucleus (in the evaporation phase), but none of these alphas is identified as the initial incident one; nor, in any case, are any alphas further transported (just as they are not in HET). Also, the two neutrons and the two protons of the incident alpha continue to be transported as four separate entities.

b. Other Particles. There are no other particles considered in HET/LHI that have not already been discussed under HET.

2. PARTICLE INTERACTIONS.

In this subsection we discuss the details of the model used for the LHI and of LHI-nucleus collisions; and we also discuss atomic collisions.

Briefly, the nonelastic collision of an LHI with a target nucleus is modeled as a sequence of successive independent single-nucleon-on-nucleus collisions, there being in the sequence one such collision for each nucleon in the LHI. The single-incident-nucleon collisions are treated by the HET modeling previously presented. Elastic collisions of LHI's with nuclei other than hydrogen are ignored.

a. The LHI Model. The properties of the LHI that must be specified in order to do transport are: (1) the geometrical arrangement of the nucleons of the LHI (from which may be inferred the position of each nucleon relative to the position of the LHI center of mass), (2) the direction of travel of each nucleon, and (3) the energy of each nucleon.

The LHI geometry is modeled as a line of half length $2.19 (A/2)^{1/3}$ fm (for an LHI with mass number A) with $[A/2]^*$ nucleons, considered to be points, located at each endpoint of the line and, for A odd, the odd nucleon being relegated to a given end with probability $1/2$. So, all the nucleons at a given end have precisely the same spatial location at any given time before collision with a target nucleus. Also, the location of the center of mass of the LHI is taken to be the center of the line.

The direction of travel of each nucleon of the LHI is taken to be the same as that of the center of the mass of the LHI.

The kinetic energy of each nucleon of the LHI is taken to be $(E_K - E_B)/A$ where E_K and E_B are the kinetic and binding energies, respectively, of the LHI; so each nucleon has the same kinetic energy.

b. Nuclear Collisions. Once again, it is convenient to divide the discussion according to whether $A = 1$ or $A \geq 5$ (with A being the mass number of the target nucleus). The latter case is discussed first.

(1) $A \geq 5$. Once it is determined (through the usual Monte Carlo sampling process using the macroscopic collision cross section [see Refs. 15 and 24 for details about macroscopic cross sections])

that a nonelastic collision of an LHI with a particular nucleus (with $A \geq 5$) of the material media is to take place, the collision process proceeds as follows. A point is randomly selected over a disc having radius equal to the sum of the LHI and target nucleus radii, this disc representing the projected area, in a plane perpendicular to the LHI center of mass linear trajectory, of the spherical target nucleus "augmented" by the LHI projectile; and the distance of this point from the center of the disc is taken to be the impact parameter of the incident LHI center of mass relative to the center of the target nucleus. Also, the angular orientation of the LHI "rod" is randomly sampled. By the discussion in the previous subsection, the impact parameter relative to the center of the target nucleus is then known for each nucleon of the LHI; and so are the nucleons' directions and kinetic energies.

Now the first nucleon of the LHI enters the nucleus and propagates, precisely as in HET, to the end of the cascade phase of INCE. Then the second and subsequent LHI nucleons do the same in turn. If none of the nucleons suffers an actual collision within the target nucleus, then the process is recycled until such a collision occurs. The accumulation of the results (particles produced plus residual excitation energy) over all incident nucleons is interpreted to be the result of the cascade phase that would have been induced by the incident LHI itself.

Note that each step of the sequence is independent in the sense that the modification of the nucleus by the n^{th} nucleon during its cascade process is not taken into account, so that the $(n+1)^{\text{th}}$ nucleon has its collisions governed by the same target nucleus density, momentum, and potential energy distributions as the n^{th} nucleon. This model is questionable for incident nucleons with energy ≥ 1 -2 GeV (Ref. 24, p. 162) and leads to the estimate of E_h given in Table 2. (Note, however, that the incident nucleons are spatially correlated and so are not independent in this sense.)

The cumulative cascade phase having been completed, the total remaining nuclear excitation energy is then used as input for a single evaporation phase calculation, which proceeds precisely as in HET.

Finally, by appealing to SGS, de-excitation photons may be produced after the evaporation phase is complete.

(2) $A = 1$. Once it is determined that a collision (elastic or inelastic) of an LHI with a hydrogen nucleus is to take place, the collision process proceeds as follows. Because the underlying model of a collision of an LHI with a hydrogen target nucleus assumes that only one nucleon of the LHI interacts with the target nucleus and all the others do not (these non-interacting nucleons proceeding with no change in direction and kinetic energy), it is first necessary to select the type of nucleon which actually interacts. This is done based upon the neutron/proton fraction in the LHI as well as upon the microscopic p-p and n-p cross sections at the incident nucleon energy. The interacting nucleon type having been selected, the collision is allowed to proceed precisely as in HET for the case $A = 1$.

c. Atomic Collisions. As pointed out earlier, HET/LHI allows source LHI's to experience atomic interactions from the moment they are born at the source until the instant just preceding their first nuclear collision. (Recall that deuterons, tritons, He^3 's, and alphas produced in nonelastic collisions are not transported and hence do not experience atomic interactions.)

*[x] = greatest integer $\leq x$.

The types of atomic interactions allowed for LHI's are not as diverse as those allowed in HET. That is, kinetic energy losses (via the stopping power formalism) due to excitation and ionization of the atomic electrons of the material media are considered. (Of course, the LHI's are not themselves atomically excited or ionized because they have no orbital electrons.) But multiple coulomb scattering--or any coulomb scattering at all--is not considered.

Stopping powers for LHI's are obtained by scaling the proton stopping powers employed in HET and it turns out (Refs. 15 and 24), for an LHI with A , Z and kinetic energy E , that $S_I(E, A, Z) = Z^2 S_p(E/A)$, where subscripts I and p refer to ion and proton respectively; here $S_p(E)$ is the proton stopping power $S(E)$ referred to in subsection II.3.c. From this, the mean range scales as $\bar{R}_I(E, A, Z) = (A/Z^2)\bar{R}_p(E/A)$; hence, a range-vs-energy table as per HET can be computed for each medium and LHI type. Range straggling effects can be computed from the Gaussian density with mean $\bar{R}_I$ and [square root of] variance given by $\sigma_I(E) = (A/Z^2)\sigma_p(E/A)$, where σ_p^2 is the variance σ^2 for protons discussed in subsection II.3.c.

3. PARTICLE TERMINATIONS.

All non-LHI particles considered by HET/LHI terminate in the same way that they do in HET. On the other hand, deuterons, tritons, He^3 's, and alpha particles (which are considered in HET), and other LHI's with $5 \leq A \leq 10$ (which are not considered in HET) are treated by HET/LHI as transportable intact until their first nuclear collision. So in HET/LHI, these particles are terminated as follows. If the kinetic energy falls below E_λ^I before the first nuclear

collision, the particle is considered to have come to rest; its position, direction and energy are recorded on the event history file. Also, the particle may escape from the system geometry before its first nuclear collision. If, on the other hand, the particle has its first nuclear collision, it ceases to exist intact and is certainly terminated. (Recall, however, that its constituent nucleons continue to be transported in an uncorrelated fashion.)

IV. SPALLATION GAMMA SOURCE (SGS)

This section discusses the SGS gamma-ray production code which provides the gamma-ray source arising from the de-excitation photons emitted after the evaporation phase of the INCE calculation in HET. Applicable references are 7, 8 and 26-28.

1. MODELING DETAILS

For each residual nucleus created in HET, with parameters A , Z , residual excitation energy E^* , and location $\vec{r}_0$ (and statistical weight W) written on the residual nucleus file created by HET, SGS creates at $\vec{r}_0$ one or more photons which subsequently serve (by being recorded on a gamma source file) as source photons for MORSE. The distribution of photon directions is sampled isotropically.

The number and energy of photons arising from a given residual nucleus is determined as follows:

- The discrete energy level structure $\{E_\alpha\} \alpha = 0, 1, \dots, N_{(A,Z)}$ (E_0 = ground-state energy) for nuclide (A, Z) is made available to the code as a data base.
- The nucleus is considered to be initially in discrete energy level E_j or E_{j+1} , where j is the unique integer such that $E_j \leq E^* < E_{j+1}$ and, for $E_j < E^* < E_{j+1}$ the choice between E_j or E_{j+1} is made by sampling randomly from the discrete density

$$f(E) = \begin{cases} 1 - \epsilon, & \text{if } E = E_j \\ \epsilon, & \text{if } E = E_{j+1} \end{cases}, \quad \epsilon = \frac{E^* - E_j}{E_{j+1} - E_j}$$

on $\Omega = \{E_j, E_{j+1}\}$. Denote the discretized initial energy so selected by E_{i_1} .

c. The nucleus then decays from level $E_{i_1} > E_0$ to a lower lying discrete level with energy E_{f_1} , the selection of the specific state E_f being governed only by the electric dipole transition probability $P(E_i \rightarrow E_f) \propto (E_i - E_f)^3$; that is,

$$P(E_{i_1} \rightarrow E_f) = (E_{i_1} - E_f)^3 / \sum_{F=0}^{i_1-1} (E_{i_1} - E_F)^3.$$

This gives rise to a single photon of energy $E_{i_1} - E_{f_1}$ being born isotropically at $\vec{r}_0$. (Note that angular momentum and parity selection rules are ignored in this process, so that every E_f with $F < i_1$ has nonzero probability of being the final energy. Further, mean lifetimes for transitions are ignored, so that "slow" transitions are not discriminated against.)

d. If E_{f_1} is the ground-state energy E_0 of (A, Z) then the residual nucleus photon emission process stops with one emitted photon. If, on the other hand, $E_{f_1} > E_0$ then the process in subparagraph c is repeated between initial level $E_{i_2} = E_{f_1}$ and selected final level E_{f_2} , with the emission of a second photon, having energy $E_{i_2} - E_{f_2}$, isotropically at $\vec{r}_0$.

e. The process in c is in fact carried out a total of s times, where s is uniquely determined by the conditions that $E_{i_s} > E_0$, $E_{f_s} = E_0$. So, in general, the residual nucleus photon emission process involves a cascade with s photons isotropically emitted at $\vec{r}_0$ having energies $E_{i_k} - E_{f_k}$, $k = 1, \dots, s$.

V. OBSERVATIONS

The HETC/LHI/SGS code system, while being a state-of-the-art tool for the type of problem it treats, could benefit from several possible improvements. Some of these should be obvious to readers of the previous sections.

The major obvious improvements are those associated with the recent LHI and SGS extensions of HETC. In particular, the LHI model itself and the LHI-nucleus interaction model are quite simplistic, and it appears that much work could be done here to improve matters. And, as pointed out earlier, perhaps the most serious deficiencies in SGS are the use of only electric dipole transition probabilities and the neglect of angular momentum and parity selection rules, leading to erroneous branching ratios. (See Refs. 7 and 8 for further discussion of these deficiencies.) Indeed, the PHT code (Ref. 29) written recently by R. Prael of the Los Alamos National Laboratory (LANL) goes a long way toward removing these shortfalls in SGS.

There are also less obvious improvements. The major items here are those improvements associated with the nucleon/pion-on-nucleus interaction model and with cross sections. As the reader may have inferred from Table 1, the HET code was written primarily to handle interactions in which the projectiles have kinetic energies ≥ 50 MeV and hence might not be entirely appropriate for projectiles having lower energies. The code modeling of interactions involving projectiles with such energies is questionable; and cross sections for collisions of

20-50 MeV nucleons with nuclei are generally not very well-known. On the other hand, this energy regime is very important when considering the transport of nucleons with maximal energies of $\lesssim 350$ MeV through thick targets in which a given nucleon may suffer several collisions and concomitant kinetic energy degradation. In addition to problems in this energy regime, there are also problems at higher energies with erroneous predictions of both the spectrum of high energy neutrons and the distribution of residual nuclei from collisions. These issues, and indeed the entire question of the improvement of the 1970-vintage high energy interaction modeling in HETC, are currently being addressed by E. Arthur and D. Madland at LANL (Ref. 30).

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