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MCNPX™ — THE LAHET™ / MCNP™ CODE MERGER

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The MCNP code is written and maintained by Group X–TM at Los Alamos National Laboratory. In response to the demands of the accelerator community, we have undertaken a major effort to expand the capabilities of MCNP to increase the set of transportable particles; to make use of newly evaluated high-energy nuclear data tables for neutrons, protons, and potentially other particles; and to incorporate physics models for use where tabular data are unavailable. A preliminary version of the expanded code, called MCNPX, has now been issued for testing. The new code includes all existing LAHET physics modules, and has the ability to utilize the 150-MeV data libraries that have recently been released by LANL Group T–2.

I. INTRODUCTION

High-energy particle transport applications at Los Alamos have traditionally been performed with the LAHET Code System (LCS),[1] a suite of computer codes for calculating the transport and interaction of nucleons, pions, muons, light ions, and antinucleons. The LCS consists of the Los Alamos version of the HETC Monte Carlo code;[2] the MCNP* general-purpose Monte Carlo code[3] for neutrons, photons, and electrons; and several tallying and postprocessing utilities. Normally, LAHET computes the transport of particles other than neutrons, photons, and electrons at all relevant energies, and of neutrons down to an intermediate "transition" energy, typically 20 MeV. The MCNP code is used for the transport of low-energy neutrons and of photons arising from the decay of neutral pions produced in the intranuclear cascade, from the de-excitation of residual nuclei after the evaporation phase, and from low-energy neutron inelastic scattering. This system works well for many applications, but there are fundamental limitations imposed by the separation of the transport problem into two parts. The most important limitation is the inability to perform completely coupled transport of all particles species. The parallel maintenance of supporting capabilities in the two separate codes is also a considerable burden on the code developers. The user interface also suffers increased complexity in the current system. For these and various other reasons, Groups X–TM and T–2 at Los Alamos National Laboratory have undertaken the development of a unified code system and associated evaluated data to calculate the cascade of nuclear particles in the greatest possible generality. The resulting software combines the theoretical models of the LAHET Code System with the powerful, general features of the MCNP code to provide a fully-coupled treatment of the transport problem.

The major benefits of the expanded MCNP code, called MCNPX, include the availability of the rich set of variance reduction methods of MCNP, use of MCNP's very general syntax for specifying geometry, sources, and tallies, flexible use of both physical models and evaluated nuclear data, and the provision of a framework for a more consistent treatment of the coupled cascade of nuclear particles. The code development has been managed in a modular fashion, so that the future inclusion of physics models from other code systems into MCNPX will be straightforward. MCNPX, Version 1.0,[4] is now in limited release for testing. We anticipate the release of a production version of the code by the end of Fiscal Year 97.

II. PHYSICS MODULES

All of the LAHET nuclear physics modules are included intact in MCNPX, Version 1.0. These include the Bertini[5] and ISABEL[6-7] intranuclear cascade (INC) models, the multistage pre-equilibrium exiton model,[8] the evaporation model,[9] the ORNL[10] (Oak Ridge National Laboratory) and RAL[11] (Rutherford Appelton Laboratory) models for fission induced by high-

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energy interactions, the Fermi breakup model,[12] the nucleon elastic scattering model,[13] and the gamma production[1] (PHT) models. A version of the FLUKA[14] high-energy generator is also included. The particle decay features of LAHET are also present in their entirety. Transport cross sections, where not determined by MCNPX library methods, are defined as in LAHET. The LAHET data files BERTIN and PHTLIB are now accessed by MCNPX to provide the necessary data for the included LAHET modules. Table 1 shows the list of particles capable of being transported with this release of MCNPX. This is a subset of the fully expanded MCNPX particle capability,[15] representing only the currently implemented particles in the MCNP and LAHET parts of the combined code. Both particles and antiparticles are listed, since they are treated differently by the code.

Table 1: Transportable Particles in MCNPX, Version 1.0

IPT	JAN	Particle Name	Symbol	Mass (MeV)	Default Energy Cutoff (MeV)	Mean Lifetime (×10 ns)
1	1	neutron	n	939.58	0.0	∞
1	-1	anti-neutron	n	939.58	0.0	∞
2	0	photon	p	0.0	0.001	∞
3	—	electron	e	0.511008	0.001	∞
3	—	positron	e	0.511008	0.001	∞
4	1	muon_–	|	105.658389	0.11261	219.703
4	-1	anti-muon_–	|	105.658389	0.11261	219.703
6	1	neutrino_e	u	0.0	0.0	∞
6	-1	anti-neutrino_e	u	0.0	0.0	∞
9	1	proton	h	938.27231	1.0	∞
9	-1	anti-proton	h	938.27231	1.0	∞
20	1	pi_+	\	139.56995	0.14875	2.603
20	-1	anti-pi_+	\	139.56995	0.14875	2.603
21	0	pi_0	z	134.9764	0.0	8.4E–09
22	1	k_+	k	493.677	0.52614	1.2371
22	-1	anti-k_+	k	493.677	0.52614	1.2371
23	1	k_0_short	%	497.672	0.000001	8.926E–03
24	1	k_0_long	^	497.672	0.000001	5.17
31	1	deuteron	d	1875.627	1.0	∞
32	1	triton	t	2808.951	1.0	∞
33	1	helium_3	s	2808.421	1.0	∞
34	1	alpha	a	3727.418	1.0	∞

The mean collisional energy-loss rates for charged particles other than electrons are calculated using an approximate treatment[16] based on the corresponding calculation for electrons. This treatment will be replaced with the methods from LAHET in the next version of MCNPX. The energy-loss straggling is sampled using a prototype implementation[17] of the Vavilov theory. This module will also be updated or replaced in a future version of the code.

III. EVALUATED PARTICLE-PRODUCTION DATA

An important requirement of the current code- and data-development plan is to develop the necessary tools to model transport of coupled neutral- and charged-particles below 150 MeV based on nuclear-data evaluations. This release of MCNPX partially meets that requirement. The physics capabilities of MCNP have been upgraded[18] to include the production of secondary charged particles from neutron collisions using data contained on expanded continuous-energy neutron cross-section tables.

The ENDF6 format[19] allows nuclear-data evaluators explicitly to include multiplicities and spectra of charged particles resulting from neutron reactions. Chadwick and Young have recently produced several such evaluations[20] fully utilizing the "n-particle" capabilities of the ENDF6 format and also extending the energy range of the incident particle to 150 MeV.

An expanded format for MCNP continuous-energy data tables to permit an arbitrary number of secondary-particle species has been developed. An auxiliary processing code called ADDCP has been written to create MCNP data tables in this expanded format. The current neutron data library resulting from these efforts contains cross-section tables for 15 isotopes and is described in the forthcoming Ref. 21.

In order to use these new evaluations and the corresponding data tables, the routines in MCNP for reading cross sections and for sampling secondary particles have been expanded. The modifications have been managed so that the methods applicable to neutron-induced charged-particle production are very similar to the existing methods for neutron-induced photon production. As in the existing neutron algorithm, the code performs a significant amount of pre-transport data manipulation. In particular, the list of active particle types, determined on the MODE card, is used to expunge unneeded data for the problem. Neutron heating numbers are also modified based on the charged particles to be transported.

At every neutron collision, the possibility exists to produce secondary charged particles. All data used in the sampling process are specific to the collision isotope and are evaluated at the incident neutron energy. The expected weight of a particular charged particle i is

$$\mathrm{WGT} \cdot \sigma_{\mathrm{cp},\,i}(E)/\sigma_{\mathrm{tot}}(E) ,$$

where WGT is the weight of the incident neutron, $\sigma_{\mathrm{cp},\,i}$ is the total particle-production cross section, σ_{tot} is the total neutron-interaction cross section, and E is the incident neutron energy. The number of charged particles produced is an integer (possibly 0) determined by analog sampling. If the code determines that a charged particle will be produced, it then samples the reaction responsible for that particle. There is no correlation between the reactions sampled as being responsible for the various secondary particles that may be produced as a result of a single neutron collision.

MCNPX supports several ENDF6 representations of scattered energy-angle distributions. Specifically, the following representations for secondary charged particles are allowed: tabular energy distributions, angular distributions via equally-probable cosine bins, Kalbach systematics for correlated energy-angle distributions, discrete two-body scattering, and n-body phase-space energy distributions. In all cases where necessary, kinematics algorithms currently incorporated in MCNP that are specific for neutron-in, neutron-out physics have been generalized to be appropriate for neutrons in and charged particles out. In addition, a general center-of-mass to laboratory conversion technique has been incorporated based on Ref. 22. As is currently the case for neutron production, all such conversions are based on the assumption of two-body kinematics, which is clearly only an approximation for many high-energy neutron reactions of current interest.

IV. USER INTERFACE

A great deal of the familiar MCNP user interface either remains unchanged, or is generalized in a very obvious way. For example, the MODE card now accepts any of the particle designators in the table of transportable particles. Thus for a transport problem involving neutrons, protons, deuterons, tritons, ^{3}He's, and alphas, but with no other particles of interest, one would specify

```
mode n h d t s a
```

to identify the active particles for the problem. In the absence of a particle type specified on the SDEF card, MCNPX follows the usual rule: the source is the active particle type with the lowest value of IPT. To specify a different source particle on the SDEF card, one uses the numerical value of IPT for the desired particle. Thus a proton source may be requested by

```
sdef ... par=9
```

An enhancement of this syntax allows the definition of antiparticle sources. Thus the card

```
sdef ... par=-9
```

specifies an antiproton source. The only exception to this enhancement is that positron sources have not yet been implemented.

As with neutrons and electrons (but not photons), the first entry on the PHYS:*pl* card specifies a maximum energy relevant to that particle type. If the user fails to give a maximum energy for each particle active in the problem, the code attempts to select a reasonable value, which will be the largest maximum energy given on PHYS cards for active particles. If no maxima are specified anywhere, the code will use 100 MeV. If particles are ignored during transport because of excessive energy, a warning is issued, and a diagnostic table is printed. The user should especially pay attention to the maximum energies in the case of source particle types that can decay or annihilate. Electrons are a special case in that their maximum energy is not allowed to exceed 1 GeV, which is the highest energy for which electron tables are available at the present time.

For all particle types, the second entry on the CUT:*pl* card determines the energy cutoff for that particle type. MCNPX contains an array of minimum allowed energy cutoffs, and a second array (currently identical) of default energy cutoffs for each particle type. These values are determined by considerations of the validity of the various theories as applied to the different particles, including consideration of the particle mass. If the user does not enter an energy cutoff for a given particle, then the default value is used.

MCNPX follows neutrons using either the physical models of LAHET, or the evaluated data in nuclear data tables. In the current version, this choice is made for all materials in the problem at a single energy. If the user does not specify this energy, then it is 20 MeV. However, the user can select a different transition energy below which the code will rely on tabular data by giving a value as the third entry on the PHYS:N card. This is an important feature if one is using the new 150-MeV data tables, for example. A future version of MCNPX will automatically make the distinction between tabular data and physical models in an isotope- and energy-dependent way. However, it should be emphasized that this release of the code expects *all* isotopes in the problem to have neutron data tables below the transition energy.

Tallies may be requested in the obvious way. For example, a proton surface current tally on surfaces 10 and 11 with two energy bins (and a total energy bin) would result from

```
f1:h 10 11
e1 100. 1000.
```

At present, only tally types 1, 2, and 4 are expected to work for the newly-supported particle types with IPT > 3.

Other particle-dependent input cards, including cell importances, IMP:*pl*, cell-dependent energy cutoffs, ELPT:*pl*, and energy splitting, ESPLT:*pl*, will probably work, but have not been tested. Some particle-dependent options, including exponential transform, forced collisions, weight windows, perturbations, DXTRAN, and detectors, have not yet been implemented, and should not be used.

Finally, the control of the physics options in the LAHET part of the code requires additional input syntax, consisting of four new MCNP-style input cards. Ref. 4 and the references contained therein give a thorough description of these new cards.

V. CODE VERIFICATION

As always in MCNP development, the standard set of 29 test problems are an essential part of the software quality assurance procedure. Version 1.0 of MCNPX passes 28 of the 29 test problems, as determined by the MCTL* files. The OUTP* files also agree in 28 out of 29 cases, except for trivial format changes necessary for the code to support the expanded particle set. The exceptional case is problem 17, a multigroup criticality problem. Here the random number sequence and all but two tally bins track the public code. There is reason to believe that the disagreement relates to a subtle problem in the dynamically allocated memory of MCNP. However, the discrepancy remains under investigation.

New test problems have also been created to serve as internal self-consistency checks on the algorithms implemented to create neutron-induced charged particles based on tabular data. It is possible to arrive at the total weight of each secondary charged-particle species produced (per history) by two independent means. The first is through the accounting of particle production by "tabular sampling" that is now displayed automatically in the particle summary tables. The second is by calculating FM tallies using the MT=200 series of total particle-production cross sections calculated by NJOY.[23] These methods should give equivalent, but independent, results for neutron energies above 20 MeV. Results from several such calculations will be documented in Ref. 21. The agreement between the two methods is quite good. These test problems only confirm the algorithms involved in sampling the weight of secondary charged particles; they do not validate the algorithms used to sample the secondary energy and angular distributions of such particles. Attention to this matter has been provided thus far via hand calculations and code debugging. Additional validation of these algorithms, including calculation of experimental benchmarks, is planned.

Additional test problems have been developed concentrating on the LAHET-based features of MCNPX. These problems have been chosen to test the logic for the handling of the new particle types and the interplay among transport, interaction, and decay. They have been used to observe the tracking changes as code modifications have occurred and to test the setting of defaults within the new code. Incident particles employed in the base test set include protons, neutrons, positive and negative pions, deuterons, antiprotons, and positive muons. The latter case was run as a coupled muon-electron-photon case. Since the incident energy for the base set was 256 MeV in all cases, not all physics modules were executed, notably the high-energy physics options. However, the Bertini and ISABEL intranuclear cascade models, the default evaporation and fission model, the pre-equilibrium model, the gamma de-excitation model, elastic nucleon scattering, and particle decay have been executed successfully. Complete balance has been achieved in the summary tables, including the processes of particle decay and antiparticle annihilation. Two other problems have been devised in both LCS and MCNPX forms which, over time, will lead to direct comparisons. The first is a standard LCS test problem for the neutron spectrum produced from 256-MeV protons on a stopping length ^{238}U target. The other is a calculation of the flux spectrum for protons at various depths as the particles slow down in thick aluminum. The latter problem is very sensitive to the details of the slowing-down process. The former test problem is relatively insensitive to that feature. A brief examination of Table 2, on the next page, shows that good agreement in the emitted angular neutron current is obtained.

Table 2: Energy-Integrated Neutron Current into Angular Bins

Angular Bin	LCS	MCNPX
180.0° – 155.0°	1.78946E-01 (0.0136)	1.81570E-01 (0.0136)
155.0° – 145.0°	1.62713E-01 (0.0140)	1.63831E-01 (0.0140)
145.0° – 125.0°	4.27562E-01 (0.0111)	4.28267E-01 (0.0111)
125.0° – 115.0°	2.43428E-01 (0.0125)	2.48396E-01 (0.0125)
115.0° – 62.5°	1.27044E+00 (0.0091)	1.27182E+00 (0.0093)
62.5° – 57.5°	1.14667E-01 (0.0152)	1.15524E-01 (0.0154)
57.5° – 32.5°	5.08595E-01 (0.0099)	5.07456E-01 (0.0101)
32.5° – 27.5°	8.22157E-02 (0.0171)	8.23298E-02 (0.0172)
27.5° – 0.0°	2.31732E-01 (0.0118)	2.32618E-01 (0.0119)
total	3.22030E+00 (0.0085)	3.23182E+00 (0.0086)

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