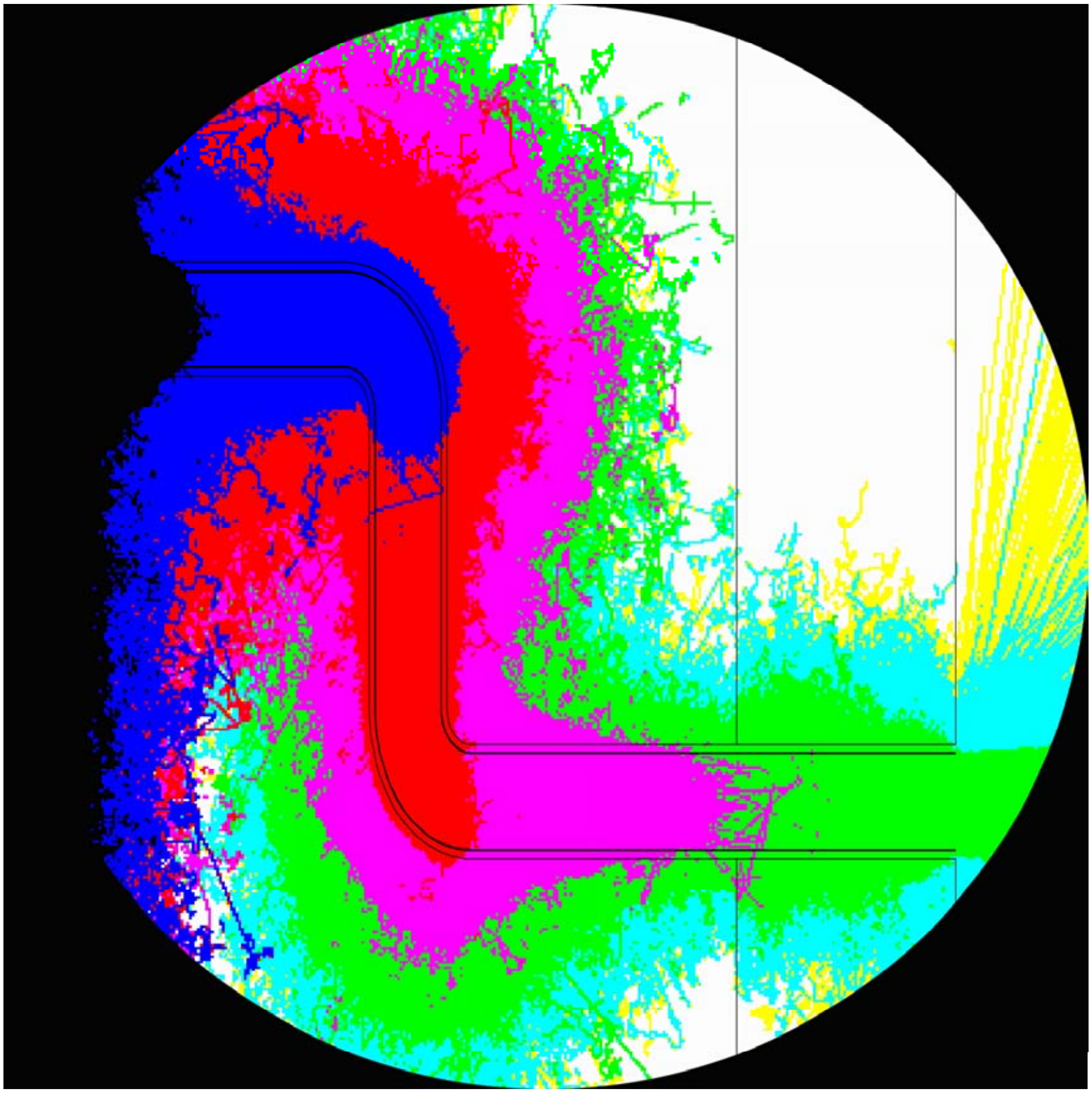
Accelerator
Production
of Tritium

MCNPX User’s Manual
Version 2.3.0, April 2002
LA-UR-02-2607



MCNPX™ USER’S MANUAL

Version 2.3.0

Laurie S. Waters, Editor

Acknowledgments

The MCNPX code and data effort represents the efforts of many people, much of whose work is represented in this manual. The primary team members are listed below.

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Beta Test Team

~800 users from 175 institutions worldwide

MCNPX was originally conceived as an upgrade to the existing Los Alamos LAHET Code System (LCS), and our deepest thanks is extended to Dr. Richard E. Prael for his support and guidance. Without his longtime vision of providing the highest quality simulation tools to the accelerator community, the MCNPX project could not have happened.

MCNPX 2.3.0 is based on MCNP4B, and we gratefully acknowledge the importance of that seminal code in our work. The MCNP code series represents many thousand person-years of effort over the past 30 years, and we hope our efforts will add new vistas to this core capability. Our special thanks goes to Dr. John Hendricks and Dr. Gregg McKinney, as well as the numerous contributors who over the years have made MCNP a world class code.

We also wish to express our appreciation to Dr. Alfredo Ferrari (currently with CERN) for allowing the use of an early version of the FLUKA code in MCNPX, permitting a significant expansion of our upper energy limits. We will endeavor in future versions of the code to upgrade this capability. In addition, we wish to express our fond appreciation for the efforts of Dr. Stepan Mashnik, who has improved the CEM code for inclusion in MCNPX.

Dr. Nikolai Mokhov of Fermi National Laboratory has provided improved high-energy photonuclear physics routines that will be implemented in future versions of the code. We also wish to thank him for his part in the formal reviews of our work.

Several visitors have provided invaluable help to the nuclear data team with evaluations, notably Dr. Satoshi Chiba (JAERI) and Dr. Arjan Koning (ECN-Petten).

We would also like to thank members of the Los Alamos Export Controls Office, particularly Sarah-Jane W. Maynard, Crystal Johnson and Steve H. Remde, for their outstanding help in dealing with the export issues for our foreign beta test team members.

Publishing Team

Finally, we wish to thank Berylene Rogers for copyediting and preparing the final document, and Patty Montoya, Barbara Olguin, Arlene Lopez, and Jean Harlow for their help in reproducing and assembling the manual.

Dedication

We dedicate this code to the memory of our respected colleague, Dr. Russell B. Kidman. Russ was an invaluable member of the APT Target/Blanket design team and a computer simulations expert for many projects at Los Alamos. His tragic and premature death has left us all with a deep sense of loss.

Contents

Figures

Tables

MCNPX User's Manual
Version 2.3.0, April 2002
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Preface

Work on the MCNPX™[1] code has been sponsored by both the Accelerator Production of Tritium (APT) and Advanced Accelerator Applications (AAA) projects in response to requests from the facility designers. Originally, MCNPX was one part of the APT effort to provide a validated set of computer simulation tools to use in design of the APT spallation target, surrounding lead blanket, and associated shielding. Other elements of this program included the production of new nuclear data evaluations from 20 to 150 MeV for neutrons, and from 1 to 150 MeV for proton and photonuclear interactions. Additional work was undertaken to provide improved total, reaction, and elastic cross section tables above 150 MeV and to improve the physics involved with the intermediate- and high-energy physics models through the CEM program. Currently the requirements of the Accelerator Transmutation of Waste program, which is part of AAA, are directed toward improvements in fission physics and actinide data.

Responsibility for the development of MCNPX was given to the APT Target/Blanket and Materials Engineering Development and Demonstration (ED&D) project. A code development team under the leadership of Dr. H. Grady Hughes was formed. Because the Los Alamos accelerator community has long supported the work of Dr. Richard Prael in the development of the LAHET™ Code System, it was decided to build on this base by combining the capabilities of LAHET and MCNP™ into one code. This involved extending the capabilities of MCNP4B™ to all particles and all energies, and including the use of physics models in the code to compute interaction probabilities where table-based data are not available.

Additional development has been provided by the theoretical efforts of the T-16 group at Los Alamos, particularly in the areas of nuclear data evaluation and expansion of physics-based models. A program of experimental activities was also undertaken, including measurement of various cross sections and development of more complex benchmarks specific to the APT and AAA projects.

Our commitment to modern software management and quality assurance methods in the development of MCNPX is very strong. The code is used for the design of high-intensity accelerator category 2 nuclear facilities, and has already been used to design a major category 3 activity at the LANSCE high-power beamstop. MCNPX development is guided by a set of requirements, design, and functional specification documents. Code testing is performed on a large scale by a volunteer beta test team. Code configuration management is

[1] MCNPX, MCNP, MCNP4B, LAHET, and LAHET Code System (LCS) are trademarks of the Regents of the University of California, Los Alamos National Laboratory.

involves the CVS system, and methods of assessing code development progress are being implemented. Training courses are held regularly. This manual has been developed to support the latest MCNPX version 2.3.0 RSICC release as an updated of the previously released document for version 2.1.5.

Geometry, basic tally and graphical capabilities of MCNPX do not fundamentally differ from the standard MCNP4B code as released to RSICC in March 1997. The MCNPX manual should be used as a supplement to the MCNP4B manual, although some additional remarks are made on basic concepts where they might need clarification for the high-energy community. The primary purpose of the MCNPX manual is to describe the extensions and additional features incorporated that directly address the high-energy, multiparticle environment envisioned in these applications. Except where noted in Chapter 2, all of the original capabilities of MCNP are intact, and MCNPX is intended to be backward-compatible with standard MCNP input files.

MCNPX code development team is now testing a version of the code fully updated to the capabilities of MCNP4C. We are also assessing the implications of Fortran-90 conversion on all parts of the code. We anticipate release of that code version later in 2002.

The MCNPX team is actively exploring code modularity in a component-architecture format, which will enable the simple addition of new routines into the code, and also allow the code to communicate with related software applications. It will also give original authors full control of their contributions. We anticipate that this advanced version of MCNPX will be available in 2003.

It is hoped that MCNPX will be of use to the Monte Carlo radiation transport community in general. The development of the modular approach in future versions of the code will facilitate the addition of new capabilities to the base code and make this tool a flexible, reliable aid in the exploration of both traditional and new mixed-energy, multiparticle applications.

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April, 2002

1 Introduction

The MCNPX program represents a major extension of the MCNP code, putting in place the ability to track all particles at all energies. MCNPX version 2.3.0 is built on MCNP4B as released to RSICC in 1997, LAHET version 2.8, plus extensions developed in LAHET version 3.0. Additional development of the CEM code was also funded through this program, and preliminary capabilities were first included in MCNPX version 2.1.5.

The MCNPX program began in 1994, when several groups in the Los Alamos X, T and LANSCE divisions proposed a program of simulation and data tool development in support of the Accelerator Production of Tritium Project. The work involved a formal extension of MCNP to all particles and all energies, improvement of physics simulation models, extension of neutron, proton and photonuclear libraries to 150 MeV, and the formulation of new variance reduction and data analysis techniques. The proposal also included a program of cross section measurements, benchmark experiments, deterministic code development, and improvements in transmutation code and library tools through the CINDER’90 project. Since the closure of the APT project, work on the code has continued under the sponsorship of the AAA and other programs.

Since the initial release of MCNPX version 2.1 on October 23, 1997, an extensive beta-test team has been formed to test the code versions prior to official release. The initial release of MCNPX version 2.1.5 to the beta-test team occurred on May 21, 1999. Final corrections and supplements to the code were released to RSICC in November, 1999, along with the current revision 1 of the User’s Manual. Approximately 800 users in ~175 institutions worldwide have had an opportunity to test the improvements in the code leading to version 2.3.0, and to provide feedback to the developers. This process is invaluable, and we express our deepest appreciation to the participants in the beta test program.

Applications for the code among the beta-test team are quite broad and constantly developing. Examples include:

- Design of accelerator spallation targets, particularly for neutron scattering facilities.
- Investigations for accelerator isotope production and destruction programs, including the transmutation of nuclear waste.
- Research into accelerator-driven energy sources.
- Medical physics, especially proton and neutron therapy.
- Investigations of cosmic-ray radiation backgrounds and shielding for high altitude aircraft and spacecraft.

- Accelerator-based imaging technology such as neutron and proton radiography.
- Design of shielding in accelerator facilities.
- Activation of accelerator components and surrounding groundwater and air.
- Investigation of fully coupled neutron-charged particle transport for lower-energy applications.
- High-energy dosimetry and neutron detection.
- Design of neutrino experiments.
- Comparison of physics-based and table-based data.
- Charged-particle tracking in plasmas.
- Charged-particle propulsion concepts for spaceflight.
- Single-event upset in semiconductors, from cosmic rays in spacecraft or from the neutron component on the earth’s surface.
- Detection technology using charged particles (i.e., abandoned landmines).

In addition to the activities of the beta-test team, the development of MCNPX is governed by several documents, including:

- MCNPX Software Management Plan
- MCNPX Requirements
- MCNPX Design
- MCNPX Functional Specifications

Configuration management of the code is done through CVS , which allows us to conveniently track issues and changes. A computer test farm of 20 different software/hardware configurations is maintained to ensure that code development does not adversely any previously tested system. We are also constantly moving toward a modular system whereby the user may easily implement alternative physics packages (EGD01). Some restructuring of the code has already been done toward that goal, including the development of an autconfiguration system.

In addition to describing the new interaction physics, this manual contains a summary of information from recent MCNPX release notes, memos, publications and presentations. It represents the work of the code development team, the nuclear data team, the physics development team, and several outside collaborators. The manual is updated and extended with each new code release.

Not all of the capabilities of MCNP4B are fully present in MCNPX version 2.3.0, and in addition the reader must be aware of certain limitations in code usage. These items are listed in Chapter 2. Chapter 3 covers code installation, and general notes on software management.

Chapter 4 gives an overview of the new high-energy physics options in addition to discussing the extended 150 MeV nuclear data libraries and other tabular data available for MCNPX. Chapter 5 describes the extended particle set, with specific notes on particle tracking, multiple scattering and energy straggling routines.

Chapter 6 contains information on modifications and enhancements to existing MCNP4B INP input cards, while Chapter 7 covers new variance reduction techniques. Chapter 8 describes new tallying capabilities. Information supplemental to the text is included in the Appendices.

This manual is not intended to replace the existing user guides to MCNP4B (BRI97), the LAHET Code System (PRA89), nor any other manual covering incorporated physics modules. The user should become familiar with these works, which are extensively referenced.

Work is now underway to fully upgrade MCNPX to MCNP4C, and to explore the possibilities inherent in conversion to Fortran-90. Classes in MCNPX are also held on a regular basis (http://mcnpxworkshops.com).

2 Warnings, Known Bugs, and Revision Notes

Although considerable effort has gone into making MCNPX compatible with MCNP, a number of features have not yet been included in MCNPX version 2.3.0, or have not yet been adequately checked out. Many of these are works in progress, to be released in future versions. Currently inoperable features are listed as warnings below.

In addition, the user must be aware of various limitations in certain code features, in order to properly use these tools. Some of these involve long-outstanding problems yet to be resolved in the simulation community, particularly involving the extension of variance reduction techniques to charged particles. Others involve known features in MCNP which have now become more important in the high energy, charged particle environment. These are listed as caveats below. All of the items listed here form a basis for future work on MCNPX.

All computer simulation codes must be validated for specific uses, and the needs of one project may not overlap completely with the needs of other projects. It is the responsibility of the user to ensure that his or her needs are adequately identified, and that benchmarking activities are performed to ascertain how accurately the code will perform. The benchmarking process for the Accelerator Production of Tritium project is extensive, yet does not cover the entire range of possible output of MCNPX. The results of these activities will be published separately, and the code development team will strive to make available results from other projects. We also solicit your input for potential code

2.1 Warnings and Known Bugs

1. **Parallel processing in MCNPX version 2.3.0 has yet to be extended to all high energy code additions.** See Section 3.1.6 for further discussion.
2. **Pertubation methods used in MCNP have not yet been extended to the non-tabular models present in MCNPX**. In MCNPX version 2.3.0 there is a bug that can cause the code to crash if run for problems that invoke the pertubation capabilities of MCNPX4B. This will be fixed in a future version.
3. **Not all plotting features have been verified for all possible outputs.** Since no changes have been made in geometry features, the geometry plotting code works well. However we have not yet been able to check out all the many features of mcplot. The user should do reasonableness checks when using this feature. For example, cross section plotting for tables other than neutrons, photons and electrons is not yet implemented.

4. **KCODE criticality calculations have not been extended to include high-energy neutrons.** Accelerator Transmutation applications should keep criticality limitations in mind when using this feature to include high-energy neutrons in the physics-based energy region. We do not anticipate problems, since criticality issues are concerned with very low energy neutron transport, however the user should carefully check the answers for reasonableness when using this feature.
5. '**Next Event Estimators', i.e., point and ring detectors, DXTRAN and radiography tally options sometimes underpredict the true answer in MCNPX**. These tallies rely on the angular distribution data for particles produced in an interaction to predict the 'next event'. Information on these distributions is available in tabular form in the libraries. This information is not easily available in the required form from physics models used to produce secondary particles above the tabular region, therefore no next-event contributions are made. If the user is certain that all particles in the problem will be produced from collisions within the tabular energy limits, next event estimators will work well. However, next-event estimates even at energies within the tabular region are not accounted for properly if the source or collision particle is above the tabular region. Thus the answer will be underestimated. Correcting this problem is a major area of investigation for the MCNPX code developers.
6. **'Next Event Estimators', i.e., point and ring detectors, DXTRAN, and radiography tally options, will not work for charged particles in any energy region.** This is due to lack of proper algorithms which can treat the effects of charged-particle scattering in these semi-deterministic methods. We have begun research to solve this long-standing problem and will implement solutions in upcoming versions of the code.
7. **Certain Weight Window optimizations have not been fully implemented for high energy particles.**
8. **The "Mix and Match" feature has yet to be implemented.** MCNPX version 2.3.0 will not switch between table based and physics based data where a number of tables with differing upper energies are present. The switch between physics models and tabular data is made at one energy for all materials in the problem. This energy is set on the PHYS card by the user (see section 6.1.7). Therefore, it is desirable that one use a set of libraries all with the same upper energy limits. Correctly implementing this feature involves a major rewrite of data structures in MCNPX, and will be released in a future version.
9. **Charged-particle reaction products are not included for some neutron reactions below 20 MeV in the LA150N library.** In calculating total particle production cross sections, the library processing routines include only those reactions where complete angular and energy information is given for secondary products. The new 150 MeV evaluations are built 'on top' of existing ENDF and JENDL evaluations which typically go to 20 MeV. Although the 150 MeV evaluations do include the detailed secondary information in the 20-150 MeV range, the < 20 MeV data typically do not. Therefore secondary production is ignored in processing that energy range. Table 4-4 lists the actual secondary particle production thresholds in LA150N.

   Fixing this situation is non-trivial, and involves a re-evaluation of the low energy data. Improved libraries will be issued, but on an isotope-by-isotope basis.

10. **Light particle residual nuclei are not transported.** When a light charged particle is the residual nucleus in a nuclear reaction in the tabular range, those charged particles are not produced, banked, and transported in MCNPX 2.3.0. Instead, their energy is assumed to be deposited locally. For example, the residual proton from neutron elastic scattering on H-1 is not produced or transported. This will be resolved in a subsequent version of MCNPX.
11. **No explicit generation of "delta ray" knockon electrons as trackable particles is done for heavy charged particles in 2.3.0.** Delta rays will be produced for electrons.
12. **The upper energy limit for photon transport is 100 GeV, and for electron transport is 1 GeV.** This is a standard feature of MCNP4B, and has been inherited by MCNPX 2.3.0. Although adequate for most uses of MCNP4B, higher energy problems often need increased upper energy ranges, particularly at electron accelerators. Future versions of MCNPX will remove these limitations.
13. **Positrons may not be used as source particles in 2.3.0.** Correcting this involves a change in the way the particle identification numbering system is handled for electrons and positrons. Historically this has not been treated in the same way as the method used for neutrons in MCNP4B, which forms the basis for the multiparticle extension of MCNPX. This will be corrected in a future MCNPX version.
14. **Beware of the results of an F6:p tally in small cells when running a photon or photon/electron problem**. Photon heating numbers include the energy deposited by electrons generated during photon collisions, but assume that the electron energy is deposited locally. In a cell where the majority of the electrons lose all of their energy before exiting that cell, this is a good approximation. However, if the cell is thin and/or a large number of electrons are created near the cell boundary, these electrons can carry significant energy into the neighboring cell, which can result in the **F6:p** tally for this cell being too large. This is a known problem in MCNP4B, where the user is cautioned that "all energy transferred to electrons is assumed to be deposited locally". (MCNP4b manual page 2-73). In MCNPX the problem can be magnified because of the high energy nature of many applications, and also because the **F6** formalism is used in the type 3 Mesh Tally. We are investigating this issue. The user is also encouraged to carefully investigate the *F8 tally, which attempts to score energy deposition by following individual particles.
15. **Continue Runs that include Mesh Tallies must use the last available complete restart dump.** The output file for mesh tallies is not integrated into the restart dump file Runtpe. However, they are written at each dump cycle. Since the mesh tally file is overwritten at each dump, care must be taken to ensure that the files used to continue a run were generated at the same dump cycle and that the last complete dump on the Runtpe file is used.
16. **An old version of FLUKA is implemented in MCNPX version 2.3.0.** The version of FLUKA now in MCNPX is taken directly from the LAHET version 2.8 code, and is known as FLUKA87. Only the high-energy portion of FLUKA is present, to handle interactions above the INC region. This is not the latest version of FLUKA, and does not contain any of the FLUKA code improvements added since that time. See Section

4.2 for further information. The FLUKA code module will be upgraded in a future version of MCNPX.

17. **The contents of the HISTP file arising from interactions processed by the CEM module do not distinguish among evaporation particles emitted before or after fission.** All are labeled as "pre-fission." Therefore the HTAPE edits that depend on this distinction will not produce the intended output:
    - pre-fission evaporation particle production spectrum
    - post-fission evaporation particle production spectrum
    - fission precursor mass edit
18. **The CEM reaction model is of limited use when light reaction targets interact with high energy incident particles.** The Fermi-Breakup model, which usually handles the reaction dynamics of light nuclei, is not implemented into CEM in MCNPX version 2.3.0. This means that at sufficiently high energies CEM can boil off all neutrons from a nucleus and hands over an unphysical highly excited nucleus to the gamma deexitation module PHT. For Sodium such events have been identified already at 500 MeV incident energy. For heavier nuclei this limit is shifted to higher energies. This will be corrected in a future version.
19. **Specifying different densities for the same material is a fatal error**. In running a neutron only problem, one can specify cells with the same material but different densities. The scaling for such situations is always linear and adjustments are straightforward. No so for charged particles, there is a density correction in energy deposition which is not a strict linear function. In MCNP4B (which is the basis for the currently released MCNPX 2.3.0), the procedure is to search through all cells and find the first one with the material in question, and use that density for the correction factor for all cells using that material. The effect is small, so this is an adequate procedure, however MCNP does give a warning message when you encounter such situations. In MCNPX, with more charged particles and greatly expanded energy range, this formerly 'small' correction now becomes increasingly important, and the usual way of handling it is not sufficient. We have therefore decided to make using the same material with more than one density a fatal error. If you want to run the problem anyway overriding the termination, the usual MCNP4B process will be followed, but we advise against it. Instead, we recommend that different materials be defined for areas of different densities.

2.2 Release Notes

Several corrections and improvements have been made to MCNPX version 2.3.0, new features have been added to the User's Manual. These are summarized below

Chapter 2 - Warnings, Caveats and Revision Notes

- Caveat regarding overprediction of heating values with th 150 MeV neutron libraries has been removed.

- Caveats regarding KCODE, and energy straggling interpolations have been removed
- Several known bugs and warnings have been added.

Chapter 3 - MCNPX Installation

- MCNPX installation discussion has been revised to incorporate automated build system (Section 3.1)
- The Cray computer platform is no longer supported. Contact the code developers if you need to use a Cray.
- Notes on multiprocessing have been added (Section 3.1.6)

Chapter 4- Physics and Data

- Proton and photonuclear capability is added in the tabular region. (Photonuclear capability in the physics region will be included in an upcoming version). See sections 4.3.1.1 and 4.3.1.2.
- 150 MeV Neutron data libraries have been updated to include Mercury and Bismuth. A 100 MeV library on ^{9}Be has also been added.
- Charged Particle Production Threshold table added (Table 4-4)
- **Nontracking change** Higher Energy Table discussion has been updated to include barpol.dat and OLDXS information (Section 4.3.1.3) Use of the new cross sections is now the default. . This will result in a higher neutron production rate on some targets.
- Section 4.3.1.4 on Atomics Mass Tables added.
- Section 4.3.1.5 on Nuclear Structure Data Library - PHTLIB added, including discussion of alternative SPEC1 file.
- Section 4.3.2.2 revised to correct mistypes.

Chapter 5 - Multiparticle Extensions and General Tracking

- Non-tracked particles information has been included in Table 5-1, and Appendix B has been deleted.
- Mass of the neutron corrected in Table 5-1.
- Corrected the symbol for charged pions in Table 5-1 from "/" to "\"
- Section 5.3 on Energy Straggling for Heavy Charged Particles has been revised to include discussion of Vavilov tracking improvements.

Chapter 6

- Additional cards needed for photonuclear interactions are described in Section 6.1
- Discussion of PHYS, CUT_N and CUT_H, and EMAX revised in Section 6.1.7.
- A list of new, MCNPX specific cards was added to section 6.1.10
- Default parameter settings for LCA, LCB, LEA and LEB were corrected.
- ** Nontracking Change ** The default setting for IPREQ on the LCA card has been changed to 1 (Use pre-equilibrium model after intranuclear cascade). In 2.1.5, the default had been 0 (No pre-equilibrium model will be used). This change was made at the overwhelming request of the users.
- Additional NOACT options added to table 6-3, for attenuation and cross section mode.
- Examples in Section 6.3 were reformatted for greater clarity. A note regarding the difference between the 'a' value defined in the manual, and that shown in Table 10 of the MCNPX output file was included.

Chapter 7

- Mistype in SPABI corrected.

Chapter 8

- In version 2.1.5, cylindrical mesh tally grids must have an inner radius starting at a value greater than 0.0. This restriction has been removed in version 2.3.0.
- Spherical Mesh Tally option is added.
- Clarification on normalization of Mesh Tallies is added.
- GNUPLOT has been added to the supported gridconv graphics options. Appendix C, which reproduces part of gridconv has been removed.
- ** Nontracking Change ** The form of the two radiography cards has been changed. Input decks are backward compatible if the name of the card only is changed.
- A cylindrical mesh has been added for the transmitted image option.
- Section 8.3 on Energy Deposition has been extensively rewritten to clarify normalization, and to discuss handling of local energy deposition
- ** Nontracking Change ** **+F6** no longer needs the :n,p designator.
- Option ic=40 (ICRP-74 1996 ambient dose equivalent) has been added for neutrons in table 8-9 (DFACT)
- Section 8.5 adds comments on the use of the histp card.

Appendices

- Added the base case input deck to Appendix A
- The table in Appendix B was incorporated into table 5-1. Appendix B is now the HTAPE3X discussion

- Appendix C was changed to discuss the use of the XSEX3

3 MCNPX Installation

This chapter describes how to build MCNPX on a system. The system will need a C and FORTRAN-77 compiler.

MCNPX installs and runs on a variety of common Unix workstations. The Cray system is no longer supported as of version 2.3.0. Some of our supported systems include:

- IBM RS-6000 AIX
- DEC Alpha Digital Unix
- SGI IRIX 32 and 64-bit
- HP HP-UX version 10
- Sun Solaris
- Intel I386 Linux

New hardware/operating systems are being added - check with the MCNPX team to get the latest status.

The code distribution contains full source code for the MCNPX 2.3.0 system and test sets for each of the supported architectures. The CDROM also contains a recent source distribution of the GNU make utility needed to properly build the system.

3.1 MCNPX Build System

3.1.1 In the Beginning

Remember that your PATH environment variable governs the search order for finding utilities. You should be aware of the value of your PATH environment variable by issuing the following command:

```
echo $PATH
```

You may find it useful to set your PATH environment variable to a strategic search order so that the utilities that are found first are the ones you intend to use. Setting of environment variables is done differently depending upon what shell you use. Please consult the appropriate manuals for your shell. Most systems have more than one shell. Any system can have more than one version of any utility. You must know your utilities.

If you work on a UNIX or Linux operating system you can use the following inquiry commands to learn if you have more than one make utility:

```
which make
which gmake
```

Many systems come with a make utility that is provided by the vendor. On UNIX and Linux, you must use the GNU make utility and it must be version 3.76 or later. Sometimes the GNU make utility is installed in an executable file called "gmake". Sometimes system administrators make symbolic links called "make" that when resolved, invoke the "gmake" utility. You can make your own symbolic links in directories that you own and control so that when you execute the "make" command you will be executing the "make" you intend to use. You can also establish an alias in the shell runtime control file whereby any "make" command you issue actually executes "gmake." You can also substitute the "gmake" command everywhere you see the "make" command in the examples that follow.

The important point of this discussion is to know your "make" and use the right one, otherwise, this automated build system can fail.

If no "make" or "gmake" is found, you either have a PATH value problem, or you need some help from your system administrator to install GNU make.

If both "make" and "gmake" exist, query each of them to see what version you have.

```
make -v
gmake -v
```

Some vendor supplied "make" utilities do not understand the "-v" option that requests that the version number be printed. If you see an error or usage message, then your "make" is one of the vendor-supplied variety. Make sure you have GNU make version 3.76 or later installed and that it is found in your search path first. If you work on a Windows platform, this distribution is not the correct one for your needs. Please request a separate Windows distribution. Until an automated build system for Windows is created, binary images will be distributed.

3.1.2 Automated Building

The process used when building mcnpx varies greatly depending upon the following:

- hardware platform e.g. SPARC, ALPHA, I386
- operating system e.g. Solaris, Linux, HP-UX
- available compilers e.g f77/cc g77/gcc pgf77/gcc
- mcnpx program options e.g. the default path of cross sections and other data files.

In past versions of MCNPX, coping with this complex set of build options required a top-level Makefile that determined the architecture and propagated these decisions to lower-level Makefiles. It was not possible to go to some lower-level makefile (Build/lcs, Build/mcnpf, ...) and do a **make**. It was also difficult to cope with different user-level options such as the desire to include mesh tallies or to exclude mesh tallies, or to compile with or without debugging.

A problem in the MCNPX-2.1 series with the various locations of X libraries on different systems added to the desire for a more complete and dynamic build system. As more platforms, operating systems, options, and compilers were added, the complexity skyrocketed.

Users of MCNPX have had to install the code and the assorted data libraries that support it manually. In particular, the methods that the code used for locating cross section files and the binary data files used by the LCS portions of the code were different from each other and poorly documented. Users had to resort to manually editing the Fortran source to customize default directories and to making symbolic links from place to place to support finding all the different sorts of data files.

Also, in past MCNPX releases, there was only one Build directory that was hard-wired into the distribution's make procedure. This build directory held all of the compilation and linking results. This inflexibility made it difficult to build different versions of the code in one place with variations of options (debugging vs. non-debugging) or comparing different compilers (Sun f77 vs. GNU g77 on Solaris, or g77 vs. the Portland Group pgf77 on Linux).

It was determined that it would be a great advantage to users if the configuration and building process of the software could better determine the hardware platform, operating system, needed libraries, and compilers that were present and perform a more complete customization.

A utility is available, the GNU Autoconf utility, that makes this possible.

A special autoconf-generated configure script distributed with MCNPX version 2.3 will examine your computing environment, adjust the necessary parameters, then generate all Makefiles in your chosen build directory so that they all match your particular computing environment. The full structure is now in place to allow a graceful migration to individual feature tests during the autoconfiguration process in the future.

The autoconf generated configure script will search for GNU compilers first before attempting to locate any other compiler present on your computing environment. Please be aware of exactly how many Fortran and C compilers exist in your computing environment. It may be necessary to specify which Fortran and C compiler should be used. You have that power via options given to the configure script. See the --with-FC and --with-CC options later in this document.

Rather than having the one Build directory of past distributions, one is now free to create as many build directories as desired, anywhere one wants, named anything one wants. Through the use of options supplied to the configure script, one can vary the resulting generated Makefiles to match a desired configuration.

Most software packages that use autoconf have a basic build procedure that looks like:

```
gzip -dc PACKAGE.tar.gz | tar xf -
cd PACKAGE
./configure
make install
```

This method of installation works with MCNPX. However, the development team recommends a slightly different method so as not to clutter the original source tree with all the products of compiling and building.

More complex packages (The GNU C compiler suite, gcc comes to mind) warn that the simple build procedure given above is a dangerous practice, as it clutters the original source tree with generated Makefiles and compiled objects, and makes it difficult to support multiple builds with different options. They suggest using a different, initially empty directory to be the target of the configure process.

```
gzip -dc PACKAGE.tar.gz | tar xf -
mkdir Build
cd Build
PATH_OF_PACKAGE-SOURCE/configure
make install
```

The MCNPX team also makes this suggestion. Please use an empty directory somewhere other than the source distribution's location as the target of the build. It keeps the source tree clean and allows multiple builds with different options. Even if you think that you will never need additional builds, it costs nothing to have the flexibility in the future.

3.1.3 MCNPX Build Examples

We will illustrate the new configure and make procedure with two primary examples; A system manager installing the MCNPX release for a system with several users, and an individual user installing the MCNPX release for their own use. A few variations on these themes are given.

3.1.3.1 System-Wide Installation

For purposes of the first illustration, we will assume that the MCNPX 2.3 distribution has been unloaded from cdrom or fetched from the net and is in the file **/usr/local/src/mcnpx_2.3.0.tar.gz**. The system manager, logged is as **root**, will unload the distribution into **/usr/local/src/mcnpx_2.3.0**, will build the system in **/tmp/mcnpx,** will install the mcnpx executable in **/usr/local/bin**, and will install the libraries (end eventually the mcnp cross sections) into **/usr/local/lib**. Naturally, the specific name of the mcnpx distribution archive will vary depending on the version you have acquired.

The following example uses **bourne** shell commands that follow accomplish this task. If you are more familiar with **csh**, you will need to adjust things appropriately. **NOTE**: Comments about the shell commands start with the '#' character. Also, don't be alarmed by the generous amount of output from the configure and make scripts. They work hard so you don't have to.

```
# go to the installation directory
cd /usr/local/src
# Unpack the distribution. This creates the directory mcnpx_2.3.0
gzip -dc mcnpx_2.3.0.tar.gz | tar xf -
# go to /tmp and make the build directory
cd /tmp
mkdir mcnpx
# go into that working space
cd mcnpx
# execute the configure script - no special option requests for the Makefiles
# the default directory prefix is /usr/local
/usr/local/src/mcnpx_2.3.0/configure
# now make the executable mcnpx program and supporting LCS libraries
make all
# run the regression tests for your architecture
make tests
# install the executables and libraries in /usr/local
make install
# clean up. The build products are no longer needed.
cd /tmp
rm -rf mcnpx
```

3.1.3.2 System-Wide Installation With Existing Directories

The previous example might typically be used when a new installation of MCNPX is performed on a system that has no pre-existing mcnpx with which to be compatible. If a user already has mcnpx, then it may be desired to use the existing locations for the data files and cross sections. Two options to the configure process can be used to customize the locations where mcnpx and its data will be installed, and the default locations where MCNPX will find those files.

When the user wants to use the normal mcnpx directory layout of:

.../bin for executables
and
.../lib for data files

but does not wish to use the default directory **/usr/local**, then the previous example can be adjusted with additional options. In the previous example, the configure script could be given the option

```
/usr/local/src/mcnpx_2.3.0/configure --prefix=/usr/mcnpx
```

and the **make install** process would install the mcnpx binary in **/usr/mcnpx/bin** and the data files in **/usr/mcnpx/lib**. The code will use /usr/mcnpx/lib as its default location for finding the data files.

When the user has an existing directory layout that does not follow the mcnpx default, then the data path itself can be customized like this:

```
/usr/local/src/mcnpx_2.3.0/configure --libdir=/usr/mcnpx
```

which will leave the default executable location as /usr/local/bin and set the location for the data files to /usr/mcnpx.

Finally, both the **--prefix** and the **--libdir** options can be used together with the **--libdir** options taking precedence over the library directory implied by the **--prefix**.

These options should remove the need to edit paths in the source code. In fact, with support for these options, there are no longer any paths in the code to edit.

3.1.3.3 Individual Private Installation

For the purpose of the second illustration, we will look at a single non-privileged user ("Me") on a computer loading and building a private copy of the code. The local user building the private copy is username **me** whose home directory is the directory **/home/me**. The user has fetched the distribution from CDROM or from the net and has it in the file **/home/me/mcnpx_2.3.0.tar.gz**. The user will unload the distribution package into **/home/me/mcnpx_2.3.0**. The user will build the system in the same directory as the source, install the binary executable in **/home/me/bin**, and install the binary data files (and eventually the mcnp cross sections) in **/home/me/lib**. This method makes it hard to make multiple versions with different options. A better example will follow this one.

The following example uses **bourne** shell commands that follow accomplish this task. If you are more familiar with **csh**, you will need to adjust things appropriately. **NOTE**: Comments about the shell commands start with the '#' character. Also, don't be alarmed by the generous amount of output from the configure and make scripts. They work hard so you don't have to.

```
# go to your user home directory
cd /home/me/
# unpack the distribution that was copied from the net or a CDROM.
# This creates /home/me/mcnpx_2.3.0
gzip -dc mcnpx_2.3.0.tar.gz | tar xf -
# go into the unpacked distribution.
cd mcnpx_2.3.0
# execute the configure script
# the --prefix tells where to put the executables and libraries.
./configure --prefix=/home/me
# Make the executable mcnpx program, the bertin and pht libraries,
# and run the regression tests
make all; make tests
# now install the executable mcnpx program and the bertin
# and pht libraries in /home/me/bin and /home/me/lib/mcnpx
make install
```

3.1.3.4 Individual Private Installation Done Better

For a more flexible version of our second example, we will look at the same single non-privileged user ("Me") on a computer loading and building a private copy of the code. This time however, the user will use a second directory away from the mcnpx source code in which to do the build. This can be done several times in different build directories with different options such as debugging/non-debugging versions or different compiler types.

The local user building the private copy is again username **me** whose home directory is the directory **/home/me**. The user has fetched the distribution from CDROM or from the net and has it in the file **/home/me/mcnpx_2.3.0.tar.gz**. The user will unload the distribution package into **/home/me/mcnpx_2.3.0**. (With this method, the source can be anywhere as long as the user has the pathname to it.) The user will build the system in the local directory **/home/me/mcnpx**, install the binary executable in **/home/me/bin**, and install the binary data files (and eventually the mcnp cross sections) in **/home/me/lib**.

The following example uses **bourne** shell commands that follow accomplish this task. If you are more familiar with **csh**, you will need to adjust things appropriately. **NOTE**: Comments about the shell commands start with the '#' character. Also, don't be alarmed by the generous amount of output from the configure and make scripts. They work hard so you don't have to.

```
# go to your user home directory
cd /home/me/
# unpack the distribution that was copied from the net or a CDROM.
# This creates /home/me/mcnpx_2.3.0
gzip -dc mcnpx_2.3.0.tar.gz | tar xf -
# make a local directory for a build directory. Call it "mcnpx".
```

```
mkdir mcnpx
# go into that new empty working space
cd mcnpx
# execute the configure script
# the --prefix tells where to put the executables and libraries.
../mcnpx_2.3.0/configure --prefix=/home/me
# now make the executable mcnpx program and the bertin and pht libraries,
# run the tests,
# and install in /home/me/bin and /home/me/lib
make all tests install
```

3.1.3.5 Individual Private Installation - special compilers and debugging

As a final example, suppose you want basically the same thing as the previous example, but you would like to have the debug option turned on during compilation. The compiled code will go into a private local library, **/home/me/bin** but you wish to use the cross section files and LCS data files already on your system. We will assume that these data files already exist in the directory **/usr/mcnpx/data**. We will assume that the source distribution has already been unpacked by a system administrator into **/usr/local/src/mcnpx_2.3.0**.

To add a bit more complexity, assume for this example that we are building and running on a Sun Solaris system that has both the GNU g77 Fortran compiler and the vendor's commercial Fortran and C compilers installed. Systems such as Sun's Solaris and HP's HP-UX normally do not include development compilers. These compilers are usually purchased as additional items. Versions of the GNU compilers are available on the net for such systems. Thus, such systems may have the GNU compilers, the Vendor's commercial compilers, or both installed. In the previous example, the GNU g77 compiler would have been used because if it exists, g77 will be found first when searching for Fortran compilers on your system. If your system has only f77, it will be found and used. We decide to specify the Sun f77 and cc compilers over the GNU g77 and gcc compilers for this build. The **--with-LD** flag may be needed in such a case because a full installation of the GNU compiler tools can also include a GNU version of the "ld" link editor. Unfortunately, the different "ld" commands take command-line arguments whose syntax differs between the two systems. As far as is known, this ONLY affects certain experimental uses of MCNPX and should not be needed by normal users. It is shown in this example as a sample of how it is used in the few cases where it is needed.

```
# go to your user home directory
cd
# set an environment variable that identifies where the distribution lives.
# This isn't really necessary, but cuts down on typing later.
MCNPX_DIST=/usr/local/src/mcnpx_2.3.0
```

```
export MCNPX_DIST
# make a working space that reminds you it's a debug version
mkdir mcnpx-debug
cd mcnpx-debug
# execute the configure script - request debug for the Makefiles,
# also specify where to put the installed code and which compilers to use.
$MCNPX_DIST/configure --with-FC=f77 --with-CC=cc --with-LD=/usr/ccs/bin/ld --with-DEBUG --prefix=/home/me --libdir=/usr/mcnpx/data
# now make the executable mcnpx program.
# We will omit the regression tests this time, although it would be a good
# idea to run them again if different compiler optimization values are used.
make install
```

That's all there is to it! There are many other options available with this new version of mcnpx. Please read the User's Notes or the Programmer's Notes for more details.

3.1.4 Directory Reorganization

In order to accommodate the use of the autoconf utility to generate the Makefiles, it became necessary to arrange the source code and regression test directories a bit. We also added a config directory to hold autoconf related code. The new directory structure is depicted in Figure 3.1.

Each of the levels contains a collection of autoconf files and links. Removal of any of these files will break the automated configure and make capabilities.

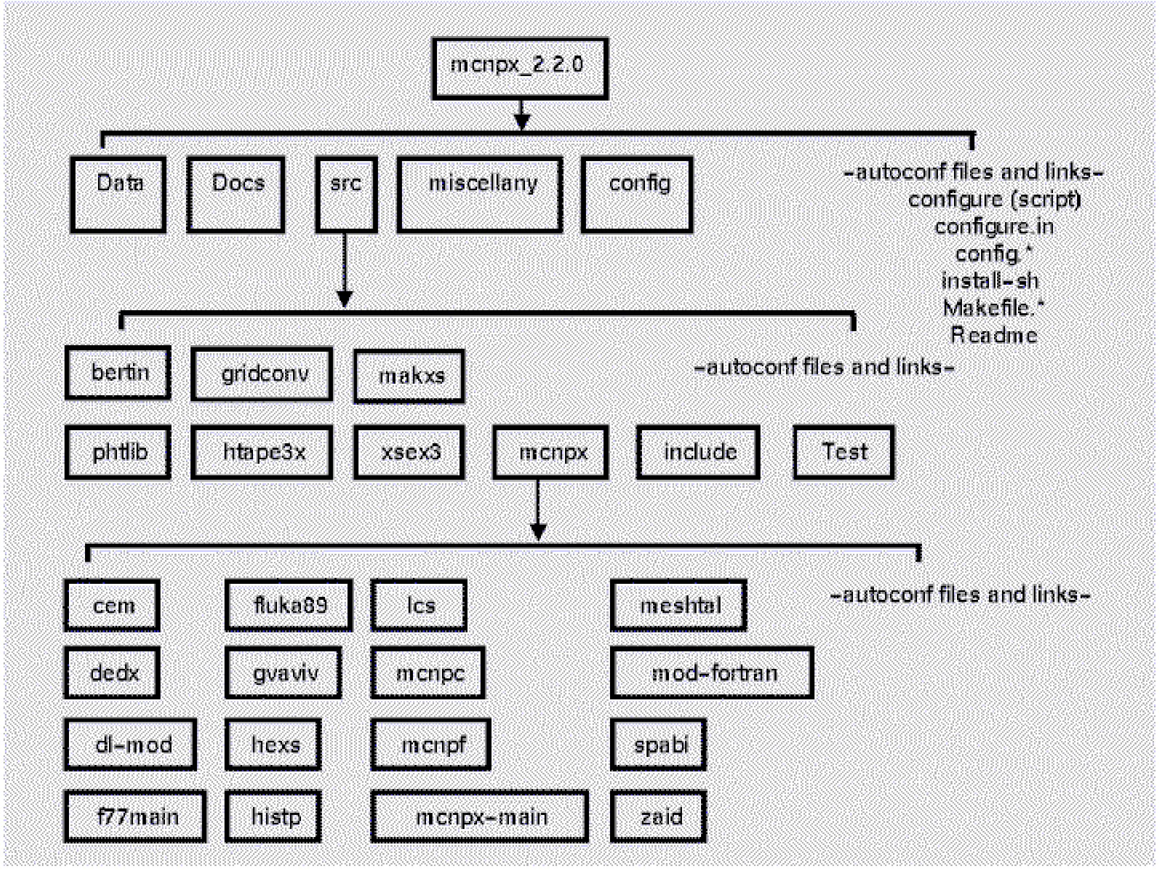
First Level: Data - contains data used with the bertin, phtlib, makexs targets Docs - contains files describing this mcnpx distribution Test - contains the regression test files for the various known platforms in use src - contains the source code files for mcnpx and several related utilities miscellany - contains things that don't fit into any other category, of interest to developers config - contains autoconf-related macros, scripts, initialization files

Second Level: bertin - builds and executes a program (hcnv) to translate LAHET text input to binary input phtlib - builds and executes a program (trx) to translate LAHET text input to binary input gridconv - converts output files generated by mesh tally and mctal files into a variety of different graphics formats htape3x - reads the history tapes (optionally generated by mcnpx) and performs post-processing on them makexs - a cross-section library management tool that converts type 1 cross-sections to type 2 cross-sections and vice versa, xsex3 - a utility associated with the new cross-section generation mode for mcnpx which allows tabulation of cross-section sets based on physics models include - contains include files shared across directories and include files localized in subdirectories mcnpx - the organizing root directory for the mcnpx program

Third Level: cem, dedx, etc. - directories that organize the Fortran77 and C source code files that are related to different aspects of the MCNPX program

Fourth Level: individual Fortran77 and C source code files for a particular aspect of MCNPX.

Figure 3.1 Directory Organization Structure



3.1.5 User's Notes

Do not edit the Makefiles generated by the configure script. In order to change the contents of the generated Makefiles, you must alter the contents of several input files that the configure script uses. Please read the Programmer's Notes in the next subsection for instructions.

Table 3.1 contains options which are available for use as parameters to the configure script for mcnpx 2.3.0

Table 3-1. Configure Script Parameters

Option Syntax	Effect on the generated Makefile if requested	Effect on the generated makefile if NOT requested
--with-STATIC	linking of the compiled files results in a static archive (mcnpx.a).	STATIC is the default - cannot be used at the same time as SHARED.
--with-SHARED	linking of the compiled files results in a dynamically linked executable (mcnpx.so).	STATIC is used - this option is exploratory for future releases of MCNPX.
--with-DEBUG	a debug switch appears in the compile step for the generated Makefiles.	no debug switch appears in the compile step for the generated Makefiles - this option can be used in combination with other options such as --with-FC and --with-CC.
--with-FC=value (substitute the desired Fortran77 compiler name for the value placeholder, e.g., --with-FC=fort to use the fort compiler)	value will be used to compile Fortran source code - location of binary directory containing value must be in your $PATH environment variable.	configure will search for a Fortran77 compiler and use the first one it finds - this option can be used in combination with other options such as --with-DEBUG and --with-CC.
--with-CC=value (substitute the desired C compiler name for the value placeholder, e.g., --with-CC=gcc to use the gcc compiler)	value will be used to compile C source code - location of binary directory containing value must be in your $PATH environment variable.	configure will search for a C compiler and use the first one it finds - this option can be used in combination with other options such as --with-DEBUG and --with-FC.
--with-LD=value (substitute the desired link editor for the value placeholder, e.g., --with-LD=/usr/ccs/bin/ld to use the Standard Sun linker)	value will be used to link object code - Unlike the --with-FC and --with-CC options, whose names are used for more than just finding the executable, The value can be a full path to the location of the desired ld program as well as being a single name like "ld".	configure will search for a linker and use the first one it finds. This is typically needed on systems with both a vendor-supplied compiler set and the GNU tool set. In such cases there may be two versions of "ld" that must be differentiated. - this option can be used in combination with other options such as --with-DEBUG and --with-FC.

Table 3-1. Configure Script Parameters

Option Syntax	Effect on the generated Makefile if requested	Effect on the generated makefile if NOT requested
--prefix=value (substitute a full path name for the value placeholder, e.g., /home/team/mcnpx) (the path given should be different from the working directory where the build is taking place)	value will be used in the install step to create bin and lib data directories for mcnpx's use.	a default value of /usr/local is used as the full path name for the install step. Executables then go to /usr/local/bin and data files go to /usr/local/lib. (permissions of the destination may prohibit success of installation).
--libdir=value (substitute a full path name for the value placeholder, e.g., /home/team/mcnpx) (the path given should be different from the working directory where the build is taking place)	value will be used in the install step to create a library data directory for mcnpx's use.	a default value of /usr/local/lib is used as the full path name for the install step (permissions of the destination may prohibit success of installation). This value overrides the library portion of the --prefix if both are given.
--with-OLDXS	the symbol OLDM is defined that is passed as -DOLDM to the compile step of mcnpx in order to activate the old cross-section capabilities.	nothing is done, new cross-section capabilities are used.
--with-no_paw or --with-no_paw=yes	this means that the symbol NO_PAW will be defined for compilation and actions are taken in the source to omit PAW capabilities when compiling.	if omitted, the default behavior is system dependent - if the detected hardware/software platform can handle PAW it is included .

Table 3-1. Configure Script Parameters

Option Syntax	Effect on the generated Makefile if requested	Effect on the generated makefile if NOT requested
--with-FFLAGS=value There is a separate variable that is used for optimization switches. See --with-FOPT in this table. If in doubt, run the configure script and examine the system default or system computed values that appear in the generated Makefile.h. You may want to include the defaults in the string you specify for FFLAGS with this mechanism when configure is run again.	substitute a quoted or double quoted string for value that represents allowable compiler switch settings - these settings will override the system default or system computed values.	if omitted, the default behavior is system dependent - the detected hardware/software platform and compilers determine what the default FFLAGS should be.
--with-CFLAGS=value There is a separate variable that is used for optimization switches. See --with-COPT in this table. If in doubt, run the configure script and examine the system default or system computed values that appear in the generated Makefile.h. You may want to include the defaults in the string you specify for CFLAGS with this mechanism when configure is run again.	substitute a quoted or double quoted string for value that represents allowable compiler switch settings - these settings will override the system default or system computed values.	if omitted, the default behavior is system dependent - the detected hardware/software platform and compilers determine what the default CFLAGS should be.
--with-FOPT=value There is a separate variable that is used for non-optimization switches. See --with-FFLAGS in this table. If in doubt, run the configure script and examine the system default or system computed values that appear in the generated Makefile.h. You may want to include the defaults in the string you specify for FOPT with this mechanism. FOPT settings are always appended to FFLAGS settings when configure is run again.	substitute a quoted or double quoted string for value that represents allowable compiler optimization switch settings - these settings will override the system default or system computed values.	if omitted, the default behavior is system dependent - the detected hardware/software platform and compilers determine what the default FOPT should be.

Table 3-1. Configure Script Parameters

Option Syntax	Effect on the generated Makefile if requested	Effect on the generated makefile if NOT requested
--with-COPT=value There is a separate variable that is used for non-optimization switches. See --with-CFLAGS in this table. If in doubt, run the configure script and examine the system default or system computed values that appear in the generated Makefile.h. You may want to include the defaults in the string you specify for COPT with this mechanism. COPT settings are always appended to CFLAGS settings when configure is run again.	substitute a quoted or double quoted string for value that represents allowable compiler optimization switch settings - these settings will override the system default or system computed values.	if omitted, the default behavior is system dependent - the detected hardware/software platform and compilers determine what the default COPT should be.

3.1.6 Multiprocessing

Many users have requested full multiprocessing, including the basic MCNP4B capability, as well as extensions to the higher energy modules unique to MCNPX. A full PVM version based on MCNPX 2.1.5 has already been prepared at Oak Ridge National Laboratory, and that version is forming the basis for formal implementation into later versions of the code. For those wishing to run with PVM, we recommend the following:

compile with option **--with-FFLAGS=”-DMULTP =DPVM**”

Unfortunately there is no --with-FLIB option for the configure script, therefore a small amount of editing must be done in Makefile.h. FLIB should be defined as:

-L/path -lfpvm -lpvm

The user is warned that multiprocessing in 2.3.0 has not yet been extended to the higher energy physics region. This is an area of active progress in code development.

3.1.7 Programmer’s Notes

Autoconf is not new; it has been available as a configuration management tool for several years. We have just recently adopted its use to simplify the build process for the mcnpx end user community, to allow the flexibility to build and keep multiple versions of mcnpx, and to improve our software development process.

3.1.7.1 Where it all starts - the relevant files - what's in them

Refer to the diagram and related description given in the figure 3.1

Table 3-2. Config Directory

File Name	Purpose
local.m4	a file containing all of the macro definitions found in the configure.in files
flags.m4ac	a file that is included in aclocal.m4, it localizes the setting of flags for different combinations of architecture, operating system, compilers
checks.m4	a file that is included in aclocal.m4, it checks for the required version of gnu make and exits with instructions if not found
configure.generic.in	a shared file used to generate configure scripts for the last level of the file tree
install-sh	a shared header file template for the Makefile that all of the levels will use
Makefile.h.in	a shared header file template for the Makefile that all of the levels will use
config.guess	a script that aids recognition of computing environments when configure is run
config.sub	a script that aids validation and canonicalization of a computing environments when configure is run

First, Second, and Third Level directories all contain special **configure.in** files that propagate the automated configuration down to the next levels. The Fourth Level directories each share the **configure.generic.in** file in the config directory because there is no further propagation.

Each of the levels (1-4) also contain a special Makefile.in and Makefile.h.in files. When the configure script runs, Makefile.h is generated, then the Makefile is generated. The first line of each Makefile includes Makefile.h.

If you make changes to any of the input files or macros, it will be necessary to regenerate the configure script so it can pick up all of the changes you have made to the component files. To regenerate the configure scripts, use the following command from the Top Level directory:

autoreconf --localdir=./config -f

This forces regeneration of the configure scripts that live at each directory level of the distribution.

The **--localdir=./config** parameter lets autoconf know where to find the macros that are called in the various **configure.in** files it encounters.

3.1.7.2 How to add a new hardware/OS/compiler

Example 1: Add the Portland Group compiler to the Linux OS on all Intel platforms (yes, it's already there, but we will step through it).

For hardware and operating system, study the case statements in the **mcnpx_2.3.0/config/config.guess** and **mcnpx_2.3.0/config/config**.sub files. You may need to insert a new case to handle your variation of hardware and operating system versions. Luckily, most of the current platforms are already specified, therefore it is unlikely that you would have to edit either of these files.

For the most recent version of autoconf, check with the <http://www.gnu.org/software/software.html#HowToGetSoftware> GNU autoconf distributions. There may be a more recent version of autoconf's config.guess/config.sub scripts that cover your configuration if it is not present in the MCNPX distribution.

Check the **config.guess** file to see if all Intel hardware platforms running Linux are specified. Several 'uname' commands at the beginning of the script set up four recognition factors that are concatenated with ':' between them (much like the setting of the PATH environment variable in some shell scripts). This concatenation of the machine, release, system, and version variables is then used in a long case statement when detecting computing platforms.

Around line 336 (in the copy current as this is being written) the ***:Linux:*:*)** case recognizes any hardware platform (not already recognized by previous cases) that run the Linux OS. Thus, no modifications are needed to config.guess.

Check the **config.sub** file to see if all Intel hardware platforms running Linux are handled in the various case statement that handle the pieces of interest. This script tries to construct and return a string that is the concatenation of cpu type, manufacturer, and operating system with the '-' character between them. Again, it is unlikely that you would have to modify this file, as most current combinations are handled. Check each of the case statements that use i[3,4,5,6] and *linux* to see if you have something different than what is specified.

For specifying a compiler in use, the **mcnpx_2.3.0/config/aclocal.m4** and the **mcnpx_2.3.0/config/flags.m4** macro definition files and the various configure.in files will be needed.

The configure.in files determine the order in which the macros in the aclocal.m4 file are activated. The order of the macro calls is very important, as some macros assume that prior work has been done. There are configure.in files in the following directories :

- configure.in in the **mcnpx_2.3.0** directory
- configure.in in the **mcnpx_2.3.0/src** directory
- configure.in in the **mcnpx_2.3.0/src/mcnpx** directory
- configure.generic.in in the **mcnpx_2.3.0/config** directory

All of the configure.in files contain the **same order of macro invocation**. The arch and system variables are set by a call to AC_SET_ARCH from configure.in.

The macro definition of AC_SET_ARCH in aclocal.m4 uses AC_CANONICAL_SYSTEM (which in turn uses config.guess and/or config.sub to do its work) to set our ARCH and SYSTEM variables. These variables are then used in combination with the FCOMP variable that specifies which Fortran compiler to use.

WARNING: Assumptions are made that an expected compatible C compiler to match the Fortran compiler has been used. You will receive warnings if the Fortran - C combination is questionable.

Find the AC_FLAGS_BY_ARCH_SYS_COMP macro call in the aclocal.m4 file. The corresponding definition for the AC_FLAGS_BY_ARCH_SYS_COMP macro is contained in its own file called **flags.m4**. The **flags.m4** file is included into the **aclocal.m4** file via the m4 include macro. Because autoconf covers (redefines) the m4 include behavior, the m4 built-in macro is used to call the m4 version of include.

Within **flags.m4** the ARCH, SYSTEM, FCOMP, CCOMP variables are used in various case statements to define needed symbols. Check to see if your arch, system, fcomp, and ccomp combination appear in this large case statement. You may need to add your combination.

For our example we are looking for usages of intel, linux, pgf77, and gcc.

Around line 21, there is a case statement that depends on the value of the ${SYSTEM} variable. We must have case label for the linux operating system. If linux did not occur, we would add it as a case and define the needed symbols that our scripts will use later when generating the various Makefile files.

Around line 70, we see a case statement that depends on the value of the ${ARCH} variable. We must have a case label for the intel hardware architecture. There is an i*86 label. The * is a wildcard character and will match a variety of intel machines (i286, i386, i486, ...). If i*86 did not appear, we would add it as a case and define the needed symbols that our scripts will use later when generating the various Makefile files.

Throughout the rest of the **flags.m4** file we find a variety of case statements that depend on the value of the ${TFC} and ${TCC} variables in combination with ${ARCH} and ${SYSTEM}. Some of these case statements are for compiler flag settings, some of these case statements are for linking the output of the compiler into executables (static and dynamic linking). These flag and option setting vary by compiler vendor and hardware platform. We must check each case statement to see if we need to add flags or options to the compile or link steps. Make sure the pgf77 (or pg*) and gcc compilers appear as case labels in these case statements and are set to your desired values.

If you add a new case label, new statements to an existing case label, or change the value of any setting, you must regenerate the configure scripts at all the different levels of the file tree hierarchy by executing the following command from within the **mcnpx_2.3.0** directory:

```
# force regeneration of configure scripts at all levels
autoreconf --localdir=./config -f
```

Once the configure scripts at the various levels have been generated, you can execute configure with the desired options that were added. For our example, we would execute the following to get our new pgf77 compiler when we make mcnpx:

```
# from the top level of your build directory
# configure and request that pgf77 be used to compile Fortran
/usr/local/src/mcnpx_2.3.0/configure --with-FC=pgf77
```

The configure will recursively descend the necessary tree hierarchy and generate Makefiles at all levels. After successful configuration you can now make mcnpx using your new compiler with the following command:

```
# from the top level of your build directory
make mcnpx
```

3.1.7.3 How to add a new feature via --with

Example 2: Add a new option to the configure script that will activate the use of the old cross-section capability during the compilation of mcnpx by defining the symbol OLDM for the compiler to recognize (yes, it's already there, but we will step through it).

This one is requires the use of **mcnpx_2.3.0/config/aclocal.m4** and **all** of the configure.in files at the various levels :

configure.in in the **mcnpx_2.3.0** directory
configure.in in the **mcnpx_2.3.0/src** directory
configure.in in the **mcnpx_2.3.0/src/mcnpx** directory
configure.generic.in in the **mcnpx_2.3.0/config** directory

Examine one of the **configure.in files.** There are several examples of checking for options, such as compiler, link method, and debug via the AC_ARG_WITH macro.

Decide where the new call to **--with-OLDXS** should be placed. Since it is only going to define one extra symbol for the compile step, it could probably be placed anywhere after the initial/default environment settings have been done (AC_CLL_DEFAULTS) and before the environment variable adjustments will be made (AC_ENV_FLAGS_VARS) for the detected and requested configuration. We placed it after the call that checks for the **--with-DEBUG** option.

The first parameter to AC_ARG_WITH is the feature you are looking for, in this case, OLDXS. Next, a descriptive string can be placed inside the quote symbols [ ]. The third parameter is the name of the macro to be executed if --with-OLDXS is given when the configure script is called. There could be fourth parameter (as in the check for the Fortran and C compilers) which is the name of the macro to be executed if the option is not given. We don't want to do anything if the --with-OLDXS option is not specified, so we don't need to supply the fourth parameter.

Go to each of the remaining **configure.in** files and place the AC_ARG_WITH call for handling --with-OLDXS in the same place as you did in the first **configure.in** file.

Now we need to define the macro that gets executed when the check for --with-OLDXS is made. We called our macro AC_SET_OLDXS. It is important to know that where we check for the presence of the parameter, and where we eventually act on the notice of its presence could be anywhere in the macros found throughout the **aclocal.m4** file. In this case, we would like to have a local variable set indicating that the option is present, then later, act on that knowledge.

In **aclocal.m4** our macro definition of AC_SET_OLDXS uses the special variable ${withval} that was set by the AC_ARG_WITH check for the presence of the option. If the option is present (= yes), then we set a local script variable, ac_oldxs, to yes. For completeness, we define that local variable with a default value of 'no' in the AC_CLL_DEFAULTS macro. This gives the variable a value even if the option was not used. Later, in a more strategic place in the code, we will test $ac_oldxs and do something appropriate.

In our case we put the code that acts to define the symbol into the AC_EXTRA_DEFINES macro, which is called last during execution of the AC_ENV_FLAGS_VARS macro. The code associated with our $ac_oldxs defines an extra symbol (OLDM) that will appear on the compile line as -DOLDM.

After saving all of the changed files, you must regenerate the configure scripts by executing the following command from within the **mcnpx_2.3.0** directory:

```
# force regeneration of configure scripts at all levels
autoreconf --localdir=./config -f
```

Once the configure scripts at the various levels have been generated, you can execute **configure** with the desired feature that were added. For our example, we would execute the following to use our new --with-OLDXS option in order to get old cross-sections activated when the Fortran code is compiled.

```
# from the top level of your working directory
# configure and request that the new option be used
configure --with-OLDXS
```

The configure will recursively descend the necessary tree hierarchy and generate Makefiles at all levels. After successful configuration you can now make mcnpx using your new compiler with the following command:

```
# from the top level of your working directory
make mcnpx
```

3.1.8 Additional Software Requirements

If you are a casual user and do not perform any software development for MCNPX capabilities, you must have the GNU make utility, version 3.76 or greater. See your system administrator if GNU make does not exist on your computing platform.

If you are a software developer for MCNPX capabilities or you wish to alter the way the autoconf generation of the configure script works, you will need the following software:

GNU make, version 3.76 or higher
GNU m4, preferably version 1.4
GNU autoconf, preferably version 2.13
GNU find, preferably version 4.1
makedepend - an X Windows routine, preferably X Version 11 Release 6

3.1.9 Fortran-90 Compilers

We have tried several Fortran 90 compilers with the default (static) construction method on several systems. The following table shows what works and what doesn't. This will change frequently, so it is best to contact the code developers for the latest results.

Table 3-3. Fortran 90 Compilers

Platform/Compiler	Result
Sun-Solaris/WorkShop Compilers 5.0 FORT90 RAN 90 2.0	core dumps
SGI-IRIX/MIPSpro Compilers: Version 7.30	terminates with errors in random places in the code
HP-HPUX/HP F90 v2.4.10	terminates with errors in random places in the code
IBM-AIX/??? (the one that came with AIX 3.4)	lots of syntax errors
Alpha-Tru64(OSF1 V5.0)/Compaq Fortran V5.3-915	works
Alpha-Linux/Compaq Fortran V1.1.0-1534 Compaq Fortran Compiler V1.1.0-1534-46B31	works, BUT behavior depends on the file suffix: .F =>FORTRAN 77 and .F90=> Fortran 90
Intel-Linux/pgf90 3.2-3	works

3.1.10 In the End...

Each subdirectory of the MCNPX distribution contains a different utility with its own install target. The top level directory also has an install target that moves into the src subdirectory and executes the install target, which covers all of the subdirectory install targets. The ultimate destination for the binary executables and associated library files depends upon what parameters were given when running the configure script. If --prefix=VALUE was given to the configure script, then the path represented by VALUE is the directory where two subdirectories shown in the table below will be created and populated. If no prefix parameter was specified for the configure, then a default directory of /usr/local is used. In both cases the bin and lib subdirectories are created and populated.

3.2 Libraries and Where to Find Them

Several types of data libraries are used by MCNPX, including the XSDIR pointer file to nuclear data tables for neutron, proton and photonuclear reactions, cross sections for the Bertini model (BERTIN), gamma emission data for decaying nuclei (PHTLIB), photon and electron interaction libraries, and others. Numerous questions in the beta test phase of

MCNPX have arisen concerning where these libraries should be kept, and this section of the manual has been added for clarification.

The following set of nuclear data libraries may be used with MCNPX 2.3.0:

1. All standard neutron libraries used with MCNP4B (DLC189) can be used with MCNPX, however they will not contain emission data for charged particles or recoil nuclei (these were processed only in the LA150N library). Therefore charged secondaries and recoil nuclei will not be produced or tracked in MCNPX within the tabular energy ranges.
2. MCNP4C (DLC200) libraries are the same as the MCNP4B DLC189 set, with certain new features. These include unresolved resonances, delayed neutrons, new electron libraries (ZAIDs end in .03e), ENDL92 data, and multi-temperature U/Np tables. DLC200 tables may be used with MCNPX, with the following cautions:

   - None of the DLC200 tables have charged particle or recoil data, therefore these will not be produced or tracked in MCNPX.
   - Only the DLC200 electron tables with ZAID numbers ending in .01e will work properly in MCNPX. .03e tables will not work. The .01e tables are included in DLC200.
   - Features related to probability tables in delayed neutrons will be ignored in MCNPX.
3. Special 150 MeV libraries (described in Section 4.3 of this manual) have been produced for use with MCNPX. The neutron library is called LA150n. The proton and photonuclear libraries are called la150h and la150u, respectively. The LA150N library is the same as DLC200, with the addition of 150 MeV evaluations above the DLC200 energy limits, and eliminating the .03e electron tables so that .01e ZAIDs are the default. Once the proton and photonuclear components are added, the entire library will be reissued under the name DLC200X.
4. A number of users are requesting secondary particle and recoil nuclei information for the lower energy portions of the libraries (typically below 20 MeV). Note that some information is available in the lower energy tables, per table 4-4 in this manual, but it is far from complete. A proper fix to the problem will involve full re-evaluations of the lower energy libraries, which is a time consuming and often difficult task. Nonetheless, progress is being made, and the user should look for improved library releases in the future.

The LANL group that formats libraries for MCNP/MCNPX is currently providing 64-bit “type 2” binary files, and MCNPX 2.3.0 will only accept these. Therefore, the user will find that older versions of 32-bit binary libraries won’t work with the 2.3.0. The program MAKXS is provided with the MCNPX distribution to do the reformatting, and details can be found in Appendix C of the MCNP4B manual. An alternative is to use “type 1” formatted, sequential access libraries.

The XSDIR file tells the code all the information it needs to known on where to find individual data tables. MCNPX uses the same procedure as MCNP4B to find the nuclear data libraries, as described in Appendix F of the MCNP4B manual. If XSDIR is not in your current directory, MCNPX will search the following places for both the libraries and XSDIR file, in order starting from #1. We repeat that portion of the MCNP4B manual here, with annotations:

1. **xsdir = "*datapath*"** on the MCNPX execution line

   note, "datapath' is truncated to 8 characters, which means that it is really the name of a file, not a path. It is easiest to assign a name via a symbolic link, e.g.:
   ln -s /home/me/lib/data/xsdir xsdir1
   Then you can say: mcnpx xsdir=xsdir1
2. **DATAPATH = *datapath*** in the INP file message block

   this version of datapath can be a full description
3. the current directory
4. the **DATAPATH** entry on the first line of the XSDIR file
5. the UNIX environmental variable: **setenv DATAPATH *datapath***
6. the individual data table line in the XSDIR file
7. the directory specified at MCNPX compile time in the blkdat.f BLOCK DATA subroutine. This can be edited to change the directory, but the code must be recompiled.

The actual coding in MCNP4B for this is a bit complex. Upon detailed examination, the MCNPX team has come up with the following slightly modified set of directions:

In the following cases, if the desired file is found, exit the list with the success.

1. Look in the current working directory for the file.
2. Look at the **DATAPATH**= input directive or the **DATAPATH** environment variable.
   - 2a. If there is a **DATAPATH**= directive in the input file, look there for the file.
   - 2b. If there was no **DATAPATH**= directive then examine the **DATAPATH** environment variable for a value.
     - 2b-1. If there is an environment value, use that value as a directory to search for the file.
     - 2b-2. If there is no value (environment variable not set) then look for the file again in the current working directory.
3. Look in a default place.
   - 3a. If there was a **DATAPATH**= directive, then the default place is either the value of the **DATAPATH** environment variable, if there was one, or value of the preprocessor symbol **LIBPREFIX** from the autoconfiguration process (typically /usr/local/lib/mcnpx).
   - 3b. If there was not a **DATAPATH**= directive in the input file, then the default is just the **LIBPREFIX** pre-processor symbol.
4. If the file is not found by now, then it is a fatal error.

The MCNPX teams plans to try and clarify this in the code for a future version.

It is recommended that MCNPX be run with 64 bit libraries. Earlier versions of the code could use 32 bit libraries, however studies of long problems have shown that erroneous answer can result with the lesser accuracy data. Conversion of Type 1 libraries to 64 bit binaries can be done with the MAKXSF routine described in Appendix C of the MCNP4B manual.

The LAHET physics modules in MCNPX require three special libraries:

BERTIN (containing the elemental cross section data needed by the Bertini model),
PHTLIB (containing nuclear structure data needed to generate de-excitation photons)
BARPOL.DAT (containing new high energy total, reaction and elastic cross sections).

They are unpacked with the rest of the code, and if ‘make install’ is executed, placed in the /lib directory. There are basically 2 ways that the code tries to find these files:

1. MCNPX tries to open the files named “bertin” and “phtlib” in the current directory. If the user wants to keep these file in another directory, a symbolic link should be made from whatever directory you are in when running the code. The following unix command can be used to do this:

   ln -s .../home/me/lib bertin
2. A default pathname is coded in the fortran data statements in the file “.../src/lcs/inbd.F”. This can be changed by the user, but you must remember to recompile the code. Look for the variable currently holding the string “/usr/local/xcodes3/lcsdir/bertin” and the similar variable referencing a location for “phtlib”. Change them to reflect the appropriate location of the two data files on your system and re-make the code. A typical location for these two files might be “/usr/local/lib/mcnpx”. This would be the preferable method when a community of users is accessing one copy of the code on a single system.

As suggested above, we recommend making a symlink to the bertin and phtlib files in your working directory. If you have more than just one person running the code from a server, then it is probably worthwhile to edit .../src/lcs/inbd.F to point to a specific location on your system where everyone can get the files, as in method 2 above. In the future we will build in the ability to look for all libraries using the same method now used for the nuclear data table libraries.

4 Physics and Data

The definitions of *low-*, *intermediate-*, and *high*-energy physics are greatly influenced by the background of the user of a simulation code. In reactor physics, a 14-MeV neutron is considered high energy, but to a particle physicist, such an energy is extremely low. There is, however, a basis for division for these categories that can be made in the context of Monte Carlo Simulation methods. Tabular data, whose evaluation contains a careful consideration of nuclear structure effects, forms a convenient area of "low" energy phenomena. In the intermediate range, above the nuclear structure region (~150 MeV in MCNPX) to a few GeV, the most common modeling methods include intranuclear/pre-equilibrium/evaporation models. Above the natural limitations of INC physics, other methods involving quantum effects are used, and MCNPX version 2.3.0 contains an early version of the FLUKA code to handle high-energy interactions.

Although our knowledge of particle physics increases constantly in sophistication, it is notable that a number of long-used techniques are still employed in the intermediate and high-energy regions. Their speed of execution is the primary factor for retention of these models. There is, however, a small but growing trend to use the more complex models to extend tabular data to high-energy regimes. In addition to improvements in computational time, an additional benefit of extended tabular data is to facilitate the use of certain variance reduction techniques at all energies. However, much research still needs to be done to validate high-energy data to the accuracy that low energy regimes can now achieve. MCNPX will be able to handle appropriately processed tabular data as it increases in upper energy limit, however we will also retain the option to use intermediate and high-energy physics modules.

The fundamentals of intermediate and high-energy physics are likely unfamiliar to most traditional users of MCNP. This chapter gives a brief explanation of the physics options offered by MCNPX in these energy regions, and also describes improvements in nuclear data libraries at lower energies. An excellent discussion of these concepts is given in FER98.

4.1 Intermediate Interaction Physics

This section gives a brief overview of the basic elements common to most intermediate energy Monte Carlo physics packages. MCNPX offers options based on three physics packages; the Bertini and ISABEL models taken from the LAHET Code System, and the CEM package, which has been specially adapted by the author for the MCNPX work. Below we describe the standard components of a physics-based package in the energy regime of ~150 MeV to a few GeV. In future versions of MCNPX it will be possible to run the code with any combination of these options, however in version 2.3.0, the components belonging to the three packages should be kept intact.

Figure 4-1 illustrates the major elements in pictorial form. In the first stage, a particle incident on a nucleus interacts with individual nucleons via particle-particle cross sections in a potential which describes the density of the nucleus as a function of radius. Intranuclear Cascade (INC) and pre-equilibrium models are used to describe this phase, in which high-energy particles and light ions are emitted, able to interact with other nuclei.

In Sections 4.1.1 through 4.1.6 we give more detail on the various physics models used to simulate these processes. Table 4-1 compares the three MCNPX options in terms of the differences in these components. Table 4-2 gives the working range of validity for each.

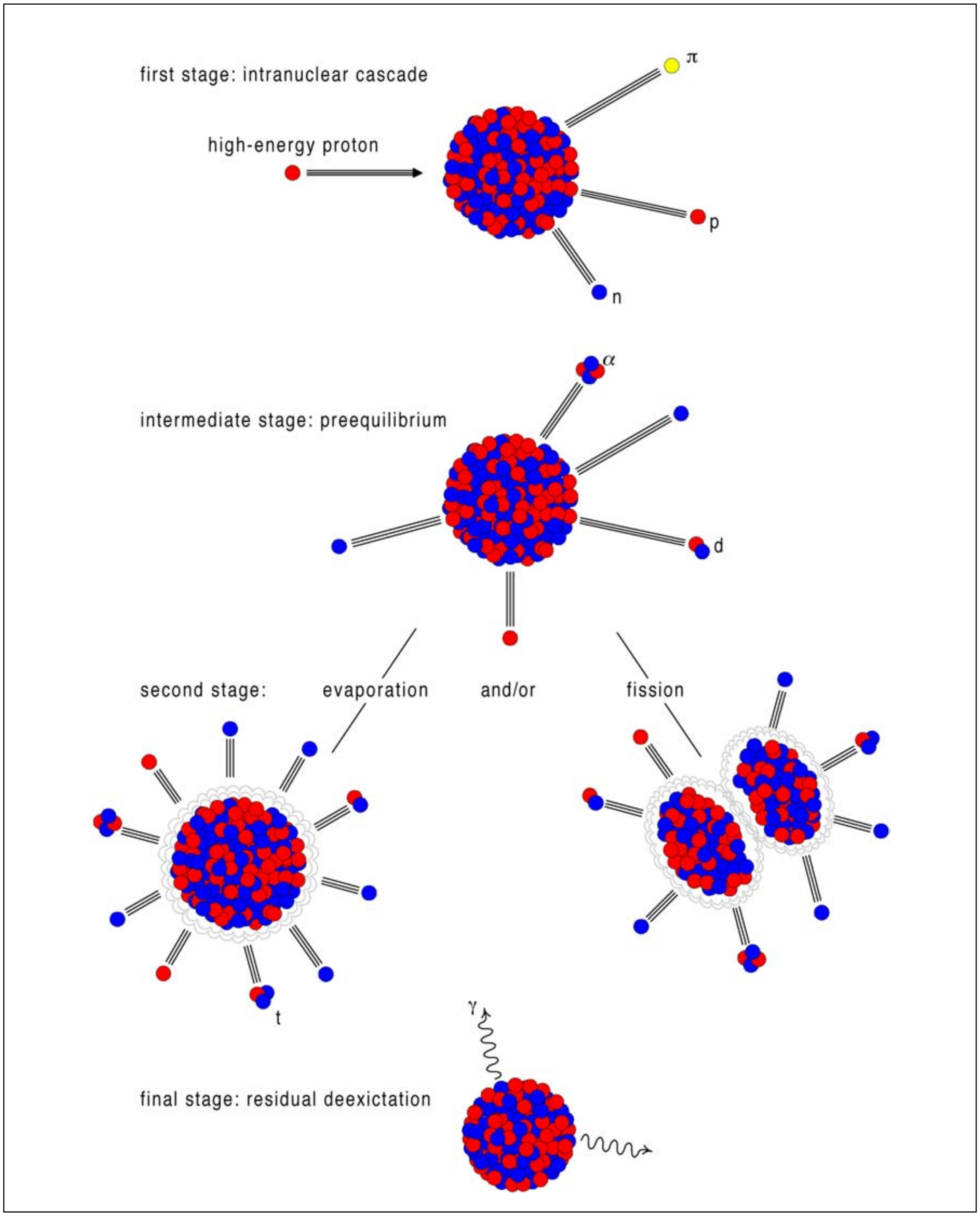

first stage: intranuclear cascade
high-energy proton
π
p
n
intermediate stage: preequilibrium
α
d
second stage:
evaporation
and/or
fission
t
γ
final stage: residual deexictation

Figure 4-1. **Interaction processes.**

Table 4-1. Summary of Physics in Intermediate Energy Models

Physics Process	Bertini	ISABEL	CEM
Method	INC + EQ or INC + PE + EQ	INC + EQ or INC + PE + EQ	INC + PE + EQ
Intranuclear Cascade Model	Bertini INC	ISABEL INC	improved Dubna INC
Monte Carlo Technique	"spacelike"	"timelike"	"spacelike"
Nuclear Density Distribution	$\rho(r)=\rho_0\{exp[(r-c)/a]+1\}$ $c=1.07A^{1/3}$ fm a=0.545 fm $\rho(r) = \alpha_i\rho(0)$; i - 1,...,3 $\alpha_1=0.9$, $\alpha_2=0.2$ $\alpha_3=0.01$	$\rho(r)=\rho_0\{exp[(r-c)/a]+1\}$ $c=1.07A^{1/3}$ fm a=0.545 fm $\rho(r) = \alpha_i\rho(0)$; i - 1,...,16	$\rho(r)=\rho_0\{exp[(r-c)/a]+1\}$ $c=1.07A^{1/3}$ fm a=0.545 fm $\rho_n(r)/\rho_p(r) = N/Z$ $\rho(r)=\alpha_i\rho(0)$; i=1,...,7 $\alpha_1=0.95$, $\alpha_2=0.8$ $\alpha_3=0.5$ $\alpha_4=0.2$ $\alpha_5=0.1$ $\alpha_6=0.05$ $\alpha_7=0.01$
Nucleon Potential	$V_N = T_F + B_N$	Nucleon kinetic energy (T_N) dependent potential $V_N=V_i(1-T_n/T_{max})$	$V_N = T_F + B_N$
Pion Potential	$V\pi = V_N$	$V\pi = 0$	$V\pi$ = 25 MeV
Mean Nucleon Binding Energy	B_N ~ 7 MeV	initial B_N from mass table; the same value is used throughout the calculation	B_N ~ 7 MeV
Elementary Cross Sections	standard BERTINI INC (old)	standard ISABEL (old)	new CEM97, last update March 1999
A + A interactions	not considered	allowed	not considered
γA interactions	not considered	not considered	may be considered
Condition for passing from the INC stage	cutoff energy ~ 7 MeV	different cutoff energies for p and n, as in VEGAS code	$P=\| (W_{mod}-W_{exp})/W_{exp} \|$ P = 0.3
Nuclear density depletion	not considered	considered	not considered
Pre-equilibrium stage	MPM (LAHET) model	MPM (LAHET) model	Improved MEM (CEM97)
Equilibrium stage	Dresner model for n, p, d, t, ^{3}He, ^{4}He emission (+ fission) (+ γ)	Dresner model for n, p, d, t, ^{3}He, ^{4}He emission (+ fission) (+ γ)	CEM97 model for n, p, d, t, ^{3}He ^{4}He emission (+ fission) (+γ)
Level density	3 LAHET models for a = a(Z, N, E*)	3 LAHET models for a = a(Z, N, E*)	CEM97 models for a = a(Z, N, E*)
Multifragmentation of light nuclei	Fermi breakup as in LAHET	Fermi breakup as in LAHET	Fermi breakup as in LAHET
Fission models	ORNL or RAL models	ORNL or RAL models	CEM model for σ_f, RAL fission fragmentation

Table 4-2. Intermediate Energy Model Recommended Ranges

Variable	Bertini	Isabel	CEM
Lower energy[a]	20 - 150 MeV	20-150 MeV	~100 MeV
Upper Energy	3.5 GeV (nucleon-nucleon 2.5 GeV (pion-nucleon)	1 GeV	5GeV
Nuclei	all	all	carbon and heavier
Incident particles	p, n, pions	A<=4 and antiprotons	p, n, pions

[a] All models will run outside their recommended energy limits; however, no detailed nuclear structure is contained at lower energies. At higher energies, the Bertini and CEM models will start to underpredict certain quantities, although 10 GeV is a reasonable upper limit.

4.1.1 Intranuclear Cascade Models

The concept of an Intranuclear Cascade (INC) model is quite old and intuitively simple.A particle incident on a nucleus will interact with individual nucleons, with final states defined by a set of fundamental particle-particle cross sections. The nucleons are considered to be a cold, free gas confined within a potential that describes the nuclear density as a function of radius, and Fermi motion of the nucleons is taken into account in modeling the interactions. In some models, the quantum effects of Pauli blocking are taken into account, however using this feature usually adds considerably to the computational time.

MCNPX offers three choices of INC models, the Bertini [BER63a, BER69], ISABEL and CEM [MAS74] packages. The Bertini model is incorporated into MCNPX through the LAHET implementation of the HETC Monte Carlo code developed at Oak Ridge National Laboratory [RAD77].

An alternative INC model was also adapted for the LAHET code from the ISABEL code [YAR78, YAR81], which allows hydrogen, helium and antiprotons as projectiles. ISABEL is derived from the VEGAS INC code [CHE68]. It has the capability of treating nucleus-nucleus interactions as well as particle-nucleus interactions (although this capability has not been yet fully tested in LAHET or MCNP). It allows for interactions between particles both of which are excited above the Fermi sea. The nuclear density is represented by up to 16 density steps, rather than the three of the Bertini INC. It also allows antiproton annihilation, with emission of kaons and pions. As presently implemented, only projectiles with A <= 4 are allowed, and antiproton annihilation is not functional. The upper incident energy limit is 1 GeV per nucleon. Running time is generally 5-10 times greater per collision than with the Bertini model.

A new third model is now offered in MCNPX version 2.3.0, the CEM code. We do note that running times for this code are long, however a new version will be issued in a future version which substantially speeds up the code.

4.1.2 Multistage Pre-equilibrium Models (MPM)

Subsequent de-excitation of the residual nucleus after the INC phase may optionally employ a multistage, multistep preequilibrium exciton model, or MPM [PRA88]. The MPM is invoked at the completion of the INC, with an initial particle-hole configuration and excitation energy determined by the outcome of the cascade. At each stage in the MPM, the excited nucleus may emit a neutron, proton, deuteron, triton, ^{3}He or alpha; alternatively, the nuclear configuration may evolve toward an equilibrium exciton number by increasing the exciton number by one particle-hole pair. The MPM terminates upon reaching the equilibrium exciton number, at which point an evaporation or Fermi-Breakup model is then applied to the residual nucleus with the remaining excitation energy.

In the LAHET/Bertini model, the inverse reaction cross sections are represented by the parameterization of Chatterjee. The potentials from which the inverse reaction cross sections are obtained are those selected by Kalbach [KAL85] for the PRECO-D2 code.

When the ISABEL intranuclear cascade model is invoked, it is possible to determine explicitly the particle-hole state of the residual nucleus since a count of the valid excitations from the Fermi sea (and the filling of existing holes) is provided. To define the initial conditions for the MPM, the number of particle-hole pairs is reduced by one for each intranuclear collision for which both exiting nucleons are below the top of the nuclear potential well. This method is the only option implemented in MCNX to link the MPM with the ISABEL INC.

In adapting the MPM to the Bertini INC, it has not been possible yet to extract the same detailed information from the intranuclear cascade history. Consequently, the algorithm which defines the interface between the Bertini INC and the MPM is a rather crude approximation, intended to permit initial evaluation of the MPM but open to further improvement. In this case, the initial condition for the MPM is one particle-hole pair beyond the minimum particle-hole configuration allowed by the outcome of the INC. The adaptive algorithm used with ISABEL is quite effective. However, given the initial condition algorithm used with the Bertini INC, the user has a choice of invoking the MPM in one of three optional modes, (or not at all):

3. The MPM continues from the final state of the INC with the initial condition defined as above (“normal MPM”).

4. The INC is used only to determine that an interaction has occurred and the MPM proceeds from the compound nucleus formed by the absorption of the incident particle ("pure MPM").
5. A random selection is made of one of the above modes at each collision with a probability P = min[E_1/E_c, 1.0] of choosing the "pure MPM" mode where E_c is the incident energy and E_1=25 MeV ("hybrid MPM").

An examination of the effect of these various options can be found in PRA94.

4.1.3 Fermi-Breakup Model

The Fermi-Breakup model [BRE81] replaces the evaporation model for the disintegration of light nuclei. It treats the deexcitation process as a sequence of simultaneous breakups of the excited nucleus into two or more products, each of which may be a stable or unstable nucleus or nucleon. Any unstable product nucleus is subject to subsequent breakup. The probability for a given breakup channel is primarily determined from the available phase space, with probabilities for two-body channels modified by Coulomb barrier, angular momentum, and isospin factors. The model is applied only for residual nuclei with A<=17, replacing the evaporation model for these nuclei. In the LAHET/MCNPX implementation, only two- and three-body breakup channels are considered; it is an abbreviated form of a more extensive implementation of the Fermi-Breakup model, with up to 7-body simultaneous breakup, used previously for cross section calculations on light nuclei [BRE89].

4.1.4 Evaporation Model

MCNPX, when used with the Bertini or ISABEL options, employs the Dresner evaporation model, based on work originally due to Weisskopf . After the INC/MPM stage, residual nuclei are in highly excited states, and energy is dissipated by evaporation of n, p, d, t, 3He and a particles. The probability p(e) that an excited nucleus will emit a particle x with kinetic energy e is proportional to :

Where S_x and m_x are the spin and mass of particle x, scx is the cross section for formation of the compound nucleus in the inverse reaction (bombarding the residual nucleus with particles of energy e), E is the excitation of the residual nucleus, and w(E) is the density of levels of the residual nucleus at excitation E. A discussion of level density options is given in section 4.1.5 below.

Although the Dresner model can emit 19 different particles from a nucleus, only those with Z up to 2 are implemented in MCNPX. The probability of emission of a particle is given by

$$R_x = (2S+1)m_x \int_{k_x V_x}^{U-Q_x-\delta} \varepsilon\sigma_{cx}(\varepsilon)\omega(U-Q_x-\delta-\varepsilon)d\varepsilon$$

Q_x is the binding energy of the particle in the nucleus, and kx are taken from inverse cross section parameterizations for each particle. V_x is the Coulomb barrier, and U is the initial excitation energy. These integrals have been solved analytically for different particles.

4.1.5 Level Densities

As the excitation energy of a nucleus increases, excited level states get closer together in energy[1]. Methods of statistical mechanics and thermodynamics have long been used to describe the structure of a highly excited nucleus. At large excitation energy E, the density of excited levels 1/D, where D is the average distance between levels, is of the form:

$$\frac{1}{D} = Ce^{2(aE)^{5^{\cdot}}}$$

where C and a are parameters which are functions of the mass number and must be empirically adjusted. Generally C is evaluated from the observed level density at low excitation (E~1 MeV), and a is adjusted to represent the spacing of levels found from the resonance capture of slow neutrons (E~6 to 8 MeV). Users of intermediate energy simulations codes have long known that results are highly sensitive to how the 'a' parameter is set. Three options for level density parameters are offered by the Bertini and ISABEL codes.

Ignatyuk model: The default evaluation of the level density parameter *a* uses the energy dependent formulation of Ignatyuk as implemented in GNASH [ART88], with the provision that:

$$\lim_{E \to 0} a(E) = a_0$$

Where E is the excitation energy and a_0 is the Gilbert-Cameron-Cook level density parameter.

[1] Excellent discussions of level density physics can be found in many standard nuclear physics textbooks, such as Chapter 11 of EVA55.

Julich model: A second model is the mass dependent model developed for the Julich version of HETC [DRE81]. In MCNPX it is applied as originally formulated, independent of energy, but could be used as the low-excitation limit in the Ignatyuk model.

HETC model: The third option is the mass and isospin dependent model originally used in the evaporation model of HETC [DRE81]:

$$a = A\frac{(1 + y_0(A - 2Z)^2)}{b_0}$$

where the default values $b_0 = 8.0$ and $y_0 = 1.5$ may be changed by the user.

4.1.6 High-Energy Fission

Two models for fission induced by high-energy interactions are included in MCNPX:

- The ORNL Model [BAR81]
- The Rutherford Appleton Laboratory (RAL) model [ATC80]

The RAL model allows fission for $Z \geq 71$ and is the default in MCNPX. It is actually two models, one for actinide and one for subactinide fission.The ORNL model covers fission only for actinides.

The subactinide fission routines of the RAL model produce cross sections which tend to be low compared to the most recent data, and use of pre-equilibrium models further reduce these values. This is strong indication that improvements in subactnide fission models are warranted.

4.2 High-Energy Interactions

MCNPX version 2.3.0 contains an early version of the FLUKA high-energy code.

Formally, this consists of the Dual Parton Model event generators HADEVT and NUCEVT [RAN85] for hadron-hadron and hadron-nucleus collisions as implemented in the form of EVENTQ in the FLUKA-87 hadron cascade code [AAR86, AAR87]. Some improvements, mainly bug corrections, were made by Ferrari and Sala in the 1989-1990 period.

Since 1987 three more FLUKA event generators have been released:

a) Release contained in GEANT versions 3.16 to 3.21, and which was contained in the official FLUKA code until Spring 1993 [FAS94a, FAS94b]

b) Release contained in the official FLUKA code until Spring 1997 [FAS97, FER98]

c) The release contained in the present version of FLUKA at this time [COL00]

4.3 Nuclear Data Tables

Tabular data is needed by MCNPX in two ways. For low energy neutrons, the usual capability of MCNP4B to use tabular data has been retained. In MCNPX this capability has been expanded to also use proton libraries, and a program is now in place to develop photonuclear capability. The collection of enhanced libraries is described in Section 4.3.1.

For interactions above library cutoff energies, additional tabular data are needed. Total, reaction and elastic cross section data are included in MCNPX in tabular format, and supplement the high-energy physics capabilities. This work is described in Section 4.3.2.

4.3.1 Nuclear Data Libraries

It has long been known that the intranuclear cascade physics includes no nuclear structure effects. Standard nuclear data libraries used with MCNP4B model such effects in detail, therefore we usually see a discontinuity in predictions in going from library upper limits to INC physics. At energies around the pion threshold[1] the simpler INC physics can adequately model reaction probabilities.

Starting in 1996, the APT project undertook the extension of standard nuclear data evaluations to 150 MeV for a number of elements of interest to the plant design. At the same time proton evaluations were also developed, and a program of photonuclear library devel-

[1] The pion production threshold is ~290 MeV for nucleons interacting with nucleons at rest. For a nucleon interacting with nucleons in a nucleus, additional Fermi energy in the nucleus lowers the threshold to ~200 MeV.

opment is underway. Since that time other programs have contributed funding for other elements. For example, the Spallation Neutron Source (SNS) program has funded the development of mercury evaluations in order to design their liquid mercury target. Programs involved in accelerator transmutation are working on actinide libraries. In contrast to previous versions, MCNPX version 2.3.0 can take full advantage of all features of the extended neutron libraries, and has added proton and photonuclear libraries. In addition, work is underway to produce libraries of certain light ion reactions. The 150 MeV libraries are released with MCNPX version 2.3.0 under the name LA150N, the proton libraries under the name LA150H, and the photonuclear libraries under LA150U.

The method for evaluating neutron-, proton-, and photon-induced cross sections uses a combination of measured cross section data and nuclear model calculations with the GNASH code. The work has been described in detail elsewhere [CHA99]. The NJOY nuclear data processing system [MAC94] is used to convert the nuclear data evaluations into a form that can be used by MCNPX. New NJOY capabilities (e.g., neutron-induced charged-particle data, incident charged-particle libraries and photonuclear libraries) have been developed within the context of NJOY99.

The full coupling of high-energy physics modules and low energy tabular data in MCNPX is still in development. The capability to use libraries which may each have different upper energy limits in one problem is referred to as the “Mix-and-Match” question. In versions 2.3.0, the switch between neutron physics models and neutron tabular data is made at one (user-specified) energy for all materials in the problem. Therefore, it is recommended that one use a set of libraries which all have upper energy limits above the user-specified value. The full coupling, which can handle the trade-off between libraries with different high-energy limits and physics modules will be released in MCNPX 3.0. The formal solution of the “Mix-and-Match” problem involves reworking of various data structures in the code. This will not be completely implemented until the end of year 2002.

4.3.1.1 The LA150 Proton and Neutron Libraries

Table 4-3 summarizes the 150 MeV neutron, proton and photonuclear libraries availble to date.

Table 4-3. Summary of LA150 Libraries

Element	Neutrons	Protons	Photonuclear[a]
Hydrogen	^{1}H, ^{2}H	^{1}H, ^{2}H	
Beryllium	^{9}Be (100 MeV)		
Carbon	^{nat}C	12C	12C
Nitrogen	^{14}N	^{14}N	
Oxygen	^{16}O	^{16}O	^{16}O

Table 4-3. Summary of LA150 Libraries (Continued)

Element	Neutrons	Protons	Photonuclear[a]
Aluminum	^{27}Al	^{27}Al	^{27}Al
Silicon	^{28}Si, ^{29}Si, ^{30}Si	^{28}Si, ^{29}Si, ^{30}Si	^{28}Si
Phosphorous	^{31}P	^{31}P	
Calcium	^{nat}Ca	^{40}Ca	^{40}Ca
Chromium	^{50}Cr, ^{52}Cr, ^{53}Cr, ^{54}Cr	^{50}Cr, ^{52}Cr, ^{53}Cr, ^{54}Cr	
Iron	^{54}Fe, ^{56}Fe, ^{57}Fe	^{54}Fe, ^{56}Fe, ^{57}Fe	^{56}Fe
Nickel	^{58}Ni,^{60}Ni,^{61}Ni,^{62}Ni,^{64}Ni	^{58}Ni,^{60}Ni,^{61}Ni,^{62}Ni,^{64}Ni	
Copper	^{63}Cu, ^{65}Cu	^{63}Cu, ^{65}Cu	^{63}Cu
Niobium	^{93}Nb	^{93}Nb	
Tantalum			^{181}Ta
Tungsten	^{182}W,^{183}W,^{184}W,^{186}W	^{182}W,^{183}W,^{184}W,^{186}W	^{184}W
Mercury	^{196}Hg, ^{198}Hg, ^{199}Hg, ^{200}Hg, ^{201}Hg, ^{202}Hg, ^{204}Hg	^{196}Hg, ^{198}Hg, ^{199}Hg, ^{200}Hg, ^{201}Hg, ^{202}Hg, ^{204}Hg	
Lead	^{206}Pb, ^{207}Pb, ^{208}Pb	^{206}Pb, ^{207}Pb, ^{208}Pb	^{206}Pb, ^{207} Pb, ^{208}Pb
Bismuth	^{209}Bi	^{209}Bi	

[a] A much larger set of photonuclear data is available at http://t2.lanl.gov/data/photonuclear.html These tables are based on IAEA Photonuclear Data Library (http://iaeand.iaea.or.at/photonuclear), and as of this writing, are available for MCNPX use on a test basis only.

Forty-two neutron evaluations have been completed for the LA150N library.The neutron evaluations are a combination of existing ENDF/B-VI Release 5 neutron evaluations up to 20 MeV, and new evaluated data from 20-150 MeV. For the mercury isotopes, the data below 20 MeV are from recent JENDL evaluations. Note, the Beryllium-9 neutron library is based on work completed 10 years ago, and only goes to 100 MeV.

Proton evaluations to 150 MeV have been completed for the same materials, except that ^{12}C and ^{40}Ca are available rather than elemental C and Ca. In contrast to the neutron evaluations, the proton work is entirely new, as no previous ENDF/B-VI “low-energy” evaluations existed upon which to build. The minimum energy of the LA150 proton evaluations ranges from 1 keV to 3 MeV. 150 MeV proton data libraries will be first distributed concurrent with the release of MCNPX version 2.3.0.

The >20 MeV neutron and all proton evaluations include:

- production cross sections for light particles
- production cross sections for gammas
- production cross sections for heavy recoil particles
- energy-angle correlated spectra for secondary light particles
- energy spectra for gammas and heavy recoil nuclei

The lower energy neutron libraries do not always contain complete secondary charged-particle emission data since they are based on earlier evaluations. In these cases, the library processing routines ignores the incomplete information. Therefore the secondary charged particles be produced and tracked below 20 MeV only for certain isotopes. Thresholds for particle emission are given in Table 4-4.

Table 4-4. Charged Particle Production Thresholds for Low Energy Neutron Libraries (MeV)

Isotope	ZAID	Proton	Deuteron	Triton	Alpha
H-1	1001.24c		1.0E-11		
H-2	1002.24c	3.339		1.0E-11	
Be-9	4009.24c	14.266	16.301	11.709	0.667
C	6000.24c	20.0	20.0		20.0
N-14	7014.24c	20.0	20.0		20.0
O-16	8016.24c	20.0	20.0		20.0
Al-27	13027.24c	1.897	6.274	11.29	3.25
Si-28	14028.24c	4.0	20.0	20.0	2.746
Si-29	14029.24c	3.0	20.0	20.0	1.3
Si-30	14030.24c	8.012	20.0	20.0	4.345
P-31	15031.24c	20.0	20.0		20.0
Ca	20000.24c	20.0	20.0	20.0	20.0
Cr-50	24050.24c	1.0	20.0	20.0	2.25
Cr-52	24052.24c	3.256	20.0	20.0	1.233
Cr-53	24053.24c	2.69	20.0	20.0	1.0
Cr-54	24054.24c	6.33	20.0	20.0	1.581
Fe-54	26054.24c	0.7	20.0	20.0	3.0
Fe-56	26056.24c	2.966	20.0	20.0	0.862

Table 4-4. Charged Particle Production Thresholds for Low Energy Neutron Libraries (MeV)

Fe-57	26057.24c	1.943	20.0	20.0	0.8
Ni-58	28058.24c	0.5	20.0	20.0	0.5
Ni-60	28060.24c	2.076	20.0	20.0	2.021E-8
Ni-61	28061.24c	0.549	20.0	20.0	0.07
Ni-62	28062.24c	4.532	20.0	20.0	0.445
Ni-64	28064.24c	6.627	20.0	20.0	2.481
Cu-63	29063.24c	0.9	20.0	20.0	1.742
Cu-65	29065.24c	1.375	20.0	20.0	0.112
Ni-93	41093.24c	20.0	20.0	20.0	20.0
W-182	74182.24c	20.0	20.0	20.0	20.0
W-183	74183.24c	20.0	20.0	20.0	20.0
W-184	74184.24c	20.0	20.0	20.0	20.0
W-186	74186.24c	20.0	20.0	20.0	20.0
Hg-196	80196.24c	20.0	20.0	20.0	20.0
Hg-198	80198.24c	20.0	20.0	20.0	20.0
Hg-199	80199.24c	20.0	20.0	20.0	20.0
Hg-200	80200.24c	20.0	20.0	20.0	20.0
Hg-201	80201.24c	20.0	20.0	20.0	20.0
Hg-202	80202.24c	20.0	20.0	20.0	20.0
Hg-204	80204.24c	20.0	20.0	20.0	20.0
Pb-206	82206.24c	20.0	20.0	20.0	20.0
Pb-207	82207.24c	20.0	20.0	20.0	20.0
Pb-208	82208.25c	4.236	5.816	6.403	1.0e-11
Bi-209	83209.24c	20.0	20.0	20.0	20.0

Note, no Helium-3 information or light ion production with Z>2 is currently available in the LA150N neutron libraries below 20 MeV.

Both the LA150 neutron and proton evaluations have also been accepted for incorporation into ENDF/B-VI as part of Release 6. A compendium [CHA99b] of neutron and proton data for most LA150 materials contains an extensive set of global, tabular and graphical representations of the new data tables.

4.3.1.2 Photonuclear Production Data

Recently work has begun on a program to evaluate photonuclear cross sections to 150 MeV for a range of materials important in accelerator components, bremsstrahlung and spallation targets, and shielding applications. Considerable interest has also been shown by researchers involved in lower energy applications, particularly the medical industry. Until now, such data have not been available in the ENDF/B-VI data library, nor have radiation transport codes such as MCNPX been able to use photonuclear data in a fully-coupled manner.

The GNASH code has been extended to include photonuclear processes, using a giant dipole resonance mechanism below 20-30 MeV, and a quasideuteron mechanism at higher energies [YOU98].Table 4-3 summarizes the currently available evaluations, which are released with MCNPX version 2.3.0. Data for all secondary particle channels are included, but particular emphasis has been placed on high-accuracy neutron production cross sections. We also note that data on photonculear interactions above 150 MeV will eventually be included in the CEM physics modules.

Work is now complete on the implementation of the new photonuclear data and physics into MCNPX version 2.3.0 [WHI99]. If photonuclear physics is enabled in a simulation (see section 6.1.7), the photon interaction cross section will be the sum of the photoatomic and the photonuclear cross sections. Full compatibility with existing MCNPX features, such as tallies, will be ensured. New summary table data are provided with relevant information about photonuclear absorption and secondary particle production.

Because photonuclear interactions are rare events, some form of biasing is useful to enable photonuclear simulations to run in a reasonable time. The concept currently implemented is similar in nature to the forced collision biassing. In forced collisions, a particle traversing a cell is split in tow; one particle is forced to undergo a collision in the material and the other is transported to the cell boundary. Both have their weights updated according to the probability that the photon would have undergone a collision before reaching the boundary. Biased photonuclear collisions borrow from this model and split the colliding photon in two, one particle undergoing a photoatomic collision, the other particle undergoing a photonuclear collisions, and both having their weights updated appropriately.

The initial challenge in making LA150 photonuclear data available for MCNPX lay in providing an interface between the data and the code. Photoatomic data tables already exist for MCNPX; one option was to append the photonuclear data to the photoatomic tables. However, photoatomic data are determined by interactions with atomic electrons, they are therefore elemental in nature. Additionally, the evaluators who work on photonuclear data are generally separate from those who work on photoatomic data. For these and other reasons it was decided to store photonuclear data for MCNPX on tables separate and distinct from the tables providing photoatomic data. A new 'u' type table has been constructed for MCNPX to hold the photnuclear data. This table follows the logic that was established for handling multiple particle emission in neutron and proton data and codifies it in a manner consistent for any incoming particle with multiple ejectiles. It uses established standard conventions for laying out the data blocks such that existing sampling algorithms can be applied.

If photonuclear physics has been enabled, in either biased or analog modes, the user must supply material descriptions that include phtonuclear tables. The standard materials (M) card has been extended to allow specification of photonuclear library IDs in the expected manner (see section 6.1.6).

Photonuclear transport using physics modules above the tabular range is available and is being tested for a near-term MCNPX release.

4.3.1.3 Higher Energy Tables

MCNPX Version 2.1.5

MCNPX includes an elastic scattering model for neutrons above 15 MeV and protons above 50 MeV, separate from the lower-energy evaluated library cross sections. The Monte Carlo methodology was adapted from the HERMES code [CLO88], with a rewritten sampling algorithm for the center-of-mass scattering angle. Elastic cross section data below 400 MeV uses a global medium-energy nucleon-nucleus phenomenological optical-model potential. This is an intermediate step in the effort to provide a library of both elastic and non-elastic cross sections from a global optical-model potential for MCNPX usage, up to ~2 GeV incident energy.

The tabulated elastic scattering cross sections were generated with an interim global medium-energy nucleon-nucleus phenomenological optical-model potential [MAD88]. The potential is based upon a relativistic Schrodinger representation and is applicable to neutron and proton incident energies in the range 50-500 MeV and a target mass of 20-220. The starting point for this work was the proton optical potential of Schwandt et. al. [SCH82], for the range 80-180 MeV.

The potential was modified to optimally reproduce experimental proton total reaction cross sections as a function of energy, while allowing only minimal deterioration in the fits to other elastic proton scattering observables. Further modifications in the absorptive potential were found necessary to extrapolate the modified potential to higher energies. At this point explicit isospin was introduced and the potential was converted to a neutron-nucleus potential by use of standard Lane model assumption and by accounting approximately for the Coulomb correction. Final comparisons of predicted and measured elastic scattering observables for both protons and neutrons were made for ^{27}Al, ^{56}Fe, and ^{208}Pb. The results were generally good.

The neutron and proton elastic cross sections so generated are tabulated for 9 mass values and 20 energies between 50 and 400 MeV. Above 400 MeV, the tabulations from HERMES are used, and the HERMES neutron elastic cross section tabulation below 50 MeV has been extended to lower and higher masses to minimize mass extrapolation error. Proton elastic scattering vanishes below 50 MeV in this implementation. Examples of the use of the elastic scattering data can be found in [PRA95].

MCNPX 2.3.0

MCNPX 2.3.0 users will notice a new file called **BARPOL.dat.** This contains improved data on reaction and elastic cross sections which is used in the ‘physics’, as opposed to the ‘library’ regions of the code. The old method described above has been retained, although the new one is the default in compiling the code. To access the old method, compile the code with the **--with-OLDXS** option from table 3-1.

Previously the concept of a reaction cross section for use with the intranuclear cascade model has been implicit in the model and not explicitly defined for use in the transport process. A new cross-section treatment [PRA98a] provides a defined (explicit) reaction cross section as well as a defined nuclear elastic cross section (previously utilized) in the absence of data libraries; these defined cross sections determine the transport process and constrain the corresponding reaction rates.

The new cross-section treatment has been implemented including an interpolation table for neutron elastic and reaction cross sections derived from the new 150-MeV MCNPX neutron libraries [CHA99a] (and some older 100-MeV libraries). Elastic scattering for protons is as implemented in LAHET2.8 [PRA96]. Proton reaction cross sections are obtained by the methods of Barashenkov and Polanski [BAR94], with Madland's optical model calculations [MAD88] used where available, augmented by the coding of Tripathi [TRI97a, TRI97b] below 1 GeV and by the methods from FLUKA89 (Moehring formulation [MOH83]) above 1 GeV. Beyond the range of the new tabular data, neutron reaction cross sections are similarly obtained. Elastic and reaction cross sections for pions are derived from the methods of Barashenkov and Polanski and of FLUKA89. For antinucleons and kaons, there are no elastic cross sections available, and the reaction cross sections are obtained only from the FLUKA89 methods.

4.3.1.4 Atomic Mass Tables

MCNPX 2.3.0 includes a new atomic mass data base [PRA98a] and the code to access it. this is used by all the physics packages shared by LAHET and MCNPX.

4.3.1.5 Nuclear Structure Data Library - PHTLIB

The PHTLIB file contains nuclear structure data used in the gamma emission process following the termination of nucleon and ion emission in residual nuclei. Two versions of PHTLIB are now available for use with MCNPX.

In the original PHTLIB released with MCNPX 2.1.5, all gamma-emitting states are allowed to decay to ground. Data was generated from CRDL structure data [HOW81]. This is a valid procedure for calculations where a source terminates and enough time has passed so that no metastable states remain. However, with new applications for transmutation of wastes, it is essential that metastable state information for residual nuclei be calculated in MCNPX for subsequent input into codes such as CINDER'90 [WIL97].

A new version of PHTLIB is now available, which not only updates the gamma emission data, and also terminates the emission process for nuclear levels with $t_{1/2}$ >= 1 nsec. The budapest_levels.dat file, compiled by G. Molnar, et. al, was obtained from the RIPL project library [CHA98] to provide the basis for the new library. Data were compared with levels in the CINDER'90 libraries, and most discrepancies resolved by reference to Firestone and Shirley [FIR96]. Improved information about low-lying levels was also added.

We have not changed the name of the new PHTLIB library, but we do recommend that you call it PHTLIB_SPEC1, and make a symbolic link in your current directory such as:

```
ln -s /home/user/data/PHTLIB_SPEC1 PHTLIB
```

Further information on the contents of the new library can be found in [PRA98c, PRA00b]. Although the new libraries do contain updated nuclear structure data, termination at 1 msec metastable states may cause confusion in interpretation of results. Careful thought should go into the decision to switch to the new library. In the future we hope to produce a method whereby the user can designate the termination time in the code.

4.3.2 Photoelectric Interactions

No change in the standard MCNP4B capability to track photoatomic interactions and electron transport has been made in MCNPX. Below we summarize part of the discussion presented in the MCNP4B manual, with comments of interest to those using these capabilities for high-energy applications. In particular, the user should be aware that the upper limit for interactions by photons is 100 GeV, and for electrons, 1 GeV. Cross sections for all photon and electron interactions are taken from the ENDF library. Part of the future work for MCNPX will be to investigate the use of the LLNL Evaluated Photon and Electron libraries, which will also raise these energy limitations.

4.3.2.1 Photon Interactions

Two physics treatments are offered, the "simple" and "detailed," as described in Part D of Chapter 2 of the MCNP4B manual. Table 4-5 summarizes the physics offered by these two options.The 'simple' physics treatment is intended for high-energy photons where little coherent scattering occurs. It is inadequate for high Z nuclides or deep penetration problems, which the user should keep in mind when performing high-energy accelerator applications.

Table 4-5. Summary of Photon Physics Options

Process	**Simple** used above energy EMCPF on the PHYS:P card (default=100 MeV)	**Detailed** used below energy EMCPF on the PHYS:P card (default=100 MeV)
Capture method	analog capture[a] used if WC1=0 on CUT:P card, otherwise implicit[b] capture used.	analog
Fluorescence	Not included	accounted for after photoelectric absorption
Photoelectric Effect	regarded as pure absorption by implicit capture. Non-captured weight undergoes either pair production or compton scattering. Capture weight is either deposited locally or becomes a photoelectron for transport.	Incident photon is absorbed, and 0 to 2 fluorescent photons emitted. An orbital electron is ejected or excited.
Pair Production Considered only in the field of a nucleus; threshold = 1.022 MeV	Same as detailed treatment.	**Mode P E**: e^+ and e^- are created, photon terminates. **Mode P with TTB**: e^+ and e^- created but not transported. Both can make TTB approximation photons. **Mode P, no TTB**: energy of e^+/e^- pair deposited locally. e^+ annihilated, replaced by two photons.
Incoherent (Compton) Scattering Klein-Nishina formula	Regarded to be on free electrons	Uses form factors to account for electron binding effects.

Table 4-5. Summary of Photon Physics Options (Continued)

Process	**Simple** used above energy EMCPF on the PHYS:P card (default=100 MeV)	**Detailed** used below energy EMCPF on the PHYS:P card (default=100 MeV)
Coherent (Thompson) Scattering Involves no energy loss, therefore no electrons are produced for further transport	Not included	Scattering angle of photon is computed, and transport continues.

a. In analog capture, a particle is killed with probability equal to the ratio of the absorption (σa) to the total cross section (σT). Killed particles deposit their entire energy and weight in the collision cell.

b. In implicit capture, the particle weight W_n is reduced to W'_n as follows: $W'_n = (1 - \sigma_a/\sigma_T) \times W_n$. If the new weight W'n is below the problem weight cutoff as specified on the CUT card, the particle is rouletted, resulting in fewer particles with larger weights. A fraction σa/σT will be deposited in the collision cell corresponding to that portion of the captured particle.

4.3.2.2 Electron Interactions

Electron transport is described in detail in Part E of Chapter 2 of the MCNP4B manual. Most users familiar with Monte Carlo techniques know that the very large number of interactions in electron transport greatly slows computational time. Therefore much work has been done to develop techniques which take advantage of the statistical nature of electron transport, assuming that the energy loss with each individual interaction is small compared to the particle's kinetic energy.In particular, energy loss and angular deflection of electrons over short steps can be sampled from probability distributions. This "condensed history" method of transport was first developed by Berger in 1963 [BER63]. Based on those techniques, Berger and Seltzer developed the ETRAN series of electron/photon transport codes [SEL88]. John Halbleib and collaborators at Sandia National Laboratory used ETRAN as the basis of the Integrated TIGER series of electron/photon transport codes [HAL88]. The electron physics in MCNP4B and MCNPX is essentially that of the Integrated TIGER series.

A brief discussion of the major physics models used in electron transport is given below. We present this detail since these or modifications of these methods are also used in heavier charged-particle transport as described in Chapter 5. This discussion is adapted from that given in Chapter 2 of the MCNP4B manual [BRI97].

Electron Collisional Stopping Power:

Berger [BER63] gives the restricted electron collisional stopping power, i.e., the energy loss per unit path length to collisions resulting in fractional energy transfers ε less than an arbitrary maximum value ε_m, in the form:

$$-\left(\frac{dE}{ds}\right)_{\varepsilon_m} = NZC\left\{\ln\left\langle E^2\frac{(\tau+2)}{2I^2}\right\rangle + f^-\ (\tau,\varepsilon_m) - \delta\right\}$$

where:

$$f^-\ (\tau,\varepsilon_m) = -1 - \beta^2 + \left(\frac{\tau}{\tau+1}\right)^2\left(\frac{\varepsilon_m^2}{2}\right) + \frac{(2\tau+1)}{(\tau+1)^2}\ln(1-\varepsilon_m) + \ln[4\varepsilon_m(1-\varepsilon_m)] + \left(\frac{1}{1-\varepsilon_m}\right)$$

Here ε and ε_m represent energy transfers as fractions of the electron kinetic energy E; I is the mean ionization potential in the same units as E; β is v/c, τ is the electron kinetic energy in units of the electron rest mass; δ is the density effect correction (related to the polarization of the medium); Z is the average atomic number of the medium; N is the atom density of the medium in cm^{-3}; and the coefficient C is given by:

$$C = \frac{(2\pi e^4)}{mv^2}$$

where m, e, and v are the rest mass, charge and speed of the electron, respectively.

The ETRAN codes and MCNP/MCNPX do not make use of restricted stopping powers, but rather treat all collisional events in an uncorrelated, probabilistic way. Thus, only the total energy loss to collisions is needed, and the above equations can be evaluated for the special value of ε_m=1/2. The reason for the 1/2 is the indistinguishability of the two outgoing electrons. The electron with the larger energy is, by definition, the primary. Therefore, only the range ε<1/2 is of interest. With ε_m=1/2, the equation for f^- becomes:

$$f^-\ (\tau,\varepsilon_m) = -\beta^2 + (1-\ln 2) + \left(\frac{1}{8} + \ln 2\right)\left(\frac{\tau}{\tau+1}\right)^2$$

On the right side, we can express both E and I in units of the electron rest mass. Then E can be replaced by τ on the right side of the equation. We also introduce supplementary constants:

$$C2 = \ln(2I^2)$$

$$C3 = 1 - \ln 2$$

$$C4 = \frac{1}{8} + \ln 2$$

so the stopping power becomes:

$$-\left(\frac{dE}{ds}\right) = NZ\frac{(2\pi e^4)}{mv^2}\left\{\ln[\tau^2(\tau+2)] - C2 + C3 - \beta^2 + C4\left(\frac{\tau}{\tau+1}\right)^2 - \delta\right\}$$

This is the collisional energy loss rate in MeV/cm in a particular medium. In MCNP/MCNPX, we are actually interested in the energy loss rate in units of MeV-barns (so that different cells containing the same material need not have the same density). Therefore, we divide this equation by N and multiply by the conversion factor, 10^{24} barns/cm^2. We also use the definition of the fine structure constant

$$\alpha = \frac{2\pi e^2}{hc}$$

where h is Planck’s constant, to eliminate the electronic charge e from the equation. The result is as follows:

$$-\left(\frac{dE}{ds}\right) = \frac{(10^{24}\alpha^2 h^2 c^2)}{2\pi mc^2}Z\left\{\ln[\tau^2(\tau+2)] - C2 + C3 - \beta^2 + C4\left(\frac{\tau}{\tau+1}\right)^2 - \delta\right\}\frac{1}{\beta^2}$$

This is the form actually used in MCNP/MCNPX to present collisional stopping powers at the energy boundaries of the major energy steps. A discussion of how collisional stopping power is implemented for heavy charged particles is found in Section 5.2.

Electron Energy Straggling:

Because an energy step represents the cumulative effect of many individual random collisions, fluctuations in the energy loss rate will occur. Thus the energy loss will not be a simple average, rather there will be a probability distribution $f(s,\Delta)d\Delta$ from which the energy loss Δ for the step of length s can be sampled. Landau [LAN44] studied this situation under the simplifying assumptions:

- The mean energy loss for a step is small compared with the electron’s energy.

- The energy parameter ξ defined below is large compared with the mean excitation energy of the medium.
- The energy loss can be adequately computed from the Rutherford cross section (RUT11).
- The formal upper limit of energy loss can be extended to infinity.

With these simplifications, Landau found that the energy loss distribution can be expressed as:

$$f(s, \Delta)d\Delta = \phi(\lambda)d\lambda$$

in terms of $\phi(\lambda)$, a universal function of a single scaled variable:

$$\lambda = \frac{\Delta}{\xi} - \ln\left[\frac{2\xi m\upsilon^2}{(1-\beta^2)I^2}\right] + \delta + \beta^2 - 1 + \gamma$$

Here, m and v are the mass and speed of the electron, δ is the density effect correction, β=v/c, I is the mean excitation energy of the medium, and γ is Euler's constant (g=0.5772157...). The parameter ξ is defined by

$$\xi = \frac{2\pi e^4 NZ}{m\upsilon^2}s$$

where e is the charge of the electron and NZ is the number density of atomic electrons, and the universal function is:

$$\phi(\lambda) = \frac{1}{2\pi i}\int_{(x-i\infty)}^{(x+i\infty)} e^{\mu\ln\mu + \lambda\mu} d\mu$$

where x is a positive real number specifying the line of integration.

Blunck and Leisegang (BLU50) have extended Landau's result to include the second moment of the expansion of the cross section. Their result can be expressed as a convolution of Landau's distribution with a Gaussian distribution:

$$f'(s, \Delta) = \frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{\infty} f(s, \Delta')\exp\left(\frac{(\Delta-\Delta')^2}{2\sigma^2}\right)d\Delta'$$

Blunck and Westphal (BLU51) provided a simple form for the variance of the Gaussian:

$$\sigma_{BW}{}^2 = 10\text{eV}Z^{\frac{4}{3}}\bar{\Delta}$$

Subsequently, Chechin and Ermilova (CHE76) investigated the Landau/Blunck-Leisegang theory, and derived an estimate for the relative error:

$$\varepsilon_{CE} \cong \left[10\frac{\xi}{I}\left(1+\frac{\xi}{10I}\right)^{3}\right]^{-\frac{1}{2}}$$

caused by the neglect of higher-order moments. Based on this work, Seltzer (SEL91) describes and recommends a correction to the Blunck-Westphal variance:

$$\sigma = \frac{\sigma_{BW}}{1+3\varepsilon_{CE}}$$

This is the value for the variance of the Gaussian which is used in MCNP/MCNPX.

Electron Multiple Scattering:

ETRAN and MCNP/MCNPX rely on the Goudsmit-Saunderson theory (GOU40) for the probability distribution of angular deflections.The angular deflection of the electron is sampled once per subset according to the distribution:

$$F(s, \mu) = \sum_{l=0}^{\infty}\left(l+\frac{1}{2}\right)\exp(-sG_l)P_l(\mu)$$

where s is the length of the substep, μ=cosϕ is the angular deflection from the direction at the beginning of the substep, $P_l(\mu)$ is the l^{th} Legendre polynomial, and G_l is:

$$G_l = 2\pi N\int_{-1}^{1}\frac{d\sigma}{d\Omega}(1-P_l(\mu))d\mu$$

in terms of the microscopic cross section $d\sigma/d\Omega$, and the atom density N of the medium.

For electrons with energies below 0.256 MeV, the microscopic cross section is taken from numerical tabulations developed from the work of Riley (RIL75).For higher-energy electrons, the microscopic cross section is approximated as a combination of the Mott (MOT29) and Rutherford cross sections (RUT11), with a screening correction. Seltzer presents this "factored cross section" in the form:

$$\frac{d\sigma}{d\Omega} = Z^2 \frac{e^2}{p^2 v^2 (1-\mu+2\eta)^2} \left[\frac{\frac{d\sigma}{d\Omega_{\mathrm{Mott}}}}{\frac{d\sigma}{d\Omega_{\mathrm{Rutherford}}}} \right]$$

where e, p and v are the charge, momentum and speed of the electron, respectively. The screening correction η was originally given by Moliere (MOL48) as:

$$\eta = \frac{1}{4}\left(\frac{\alpha mc}{0.885p}\right)^2 Z^{\frac{2}{3}}\left(1.13 + 3.76\left(\alpha\frac{Z}{\beta}\right)^2\right)$$

where α is the fine structure constant, m is the rest mass of the electron, and β=v/c. MCNP/MCNPX now follows the recommendation of Seltzer (SEL88), and the implementation in the Integrated TIGER Series, by using the slightly modified form:

$$\eta = \frac{1}{4}\left(\frac{(\alpha mc)}{0.885p}\right)^2 Z^{\frac{2}{3}}\left(1.13 + 3.76\left(\alpha\frac{Z}{\beta}\right)^2\left(\frac{\tau}{(\tau+1)}\right)^{\frac{1}{2}}\right)$$

where τ is the electron energy in units of electron rest mass. The multiplicative factor in the final term is an empirical correction which improves the agreement at low energies between the factored cross section and the more accurate partial-wave cross sections of Riley.

A discussion of the extension of this theory to heavy charged particles is found in Section 5.4.

Electron Bremsstrahlung:

MCNP and MCNP4B use the Bethe-Heitler (BET34) Born-approximation to sample bremsstrahlung photons. Formulas and approximations relevant to the present level of theory in MCNP4B and MCNPX can be found in the paper of Koch and Motz (KOC59). Particular prescriptions appropriate to Monte Carlo calculations have been developed by Berger and Seltzer (BER70). These data have been converted to tables including bremsstrahlung production probabilities, photon energy distributions and photon angular distributions, and are used directly in MCNP4B/MCNPX.

An alternative to the use of tabular data is a simple, material-independent probability distribution:

$$p(\mu)d\mu = \frac{(1-\beta^2)}{2(1-\beta\mu)^2}d\mu$$

where μ=cosϕ and β=v/c is used to sample for the angle of the photon relative to the direction of the electron according to the formula:

$$\mu = \frac{(2\varepsilon - 1 - \beta)}{(2\varepsilon\beta - 1 - \beta)}$$

where ε is a random number. This method is used for detectors and **DXTRAN** spheres where a set of source contributions p(μ) consistent with the tabular data is not available.

On should note that although bremsstrahlung for heavy charge particles is a valid physical phenomena, it is not currently implemented in MCNPX version 2.3.0. In intermediate energy physics applications this source is small, however the user should be warned that at very high energies it could become a non-negligible component.

Knock-on Electrons:

The Moller cross section for scattering of an electron by an electron is:

$$\frac{d\sigma}{d\varepsilon} = \frac{C}{E}\left(\frac{1}{\varepsilon^2} + \frac{1}{(1-\varepsilon)^2} + \left(\frac{\tau}{(\tau+1)}\right)^2 - \frac{(2\tau+1)}{(\tau+1)^2}\frac{1}{\varepsilon(1-\varepsilon)}\right)$$

where ε is the energy transfer as a fraction of electron kinetic energy E, and t is the electron kinetic energy in units of the electron rest mass. When sampling for transportable secondary particles one wants the probability of energy transfers greater than some cutoff energy ε_c below which particles will not be followed. This probability can be written:

$$\sigma(\varepsilon_c) = \int_{\varepsilon_c}^{\frac{1}{2}} \frac{d\sigma}{d\varepsilon} \mathrm{d}\varepsilon$$

The reason for the upper limit of 1/2 is the same as that given for collisional stopping power. Explicit integration of this equation gives

$$\sigma(\varepsilon_c) = \frac{C}{E}\left(\frac{1}{\varepsilon_c} - \left(\frac{1}{1-\varepsilon_c}\right) + \left(\frac{\tau}{\tau+1}\right)^2\left(\frac{1}{2} - \varepsilon_c\right) - \frac{(2\tau+1)}{(\tau+1)^2}\ln\frac{(1-\varepsilon_c)}{\varepsilon_c}\right)$$

Then the normalized probability distribution for the generation of secondary electrons with $\varepsilon > \varepsilon_c$ is given by:

$$g(\varepsilon, \varepsilon_c)\mathrm{d}\varepsilon = \frac{1}{\sigma(\varepsilon_c)}\frac{d\sigma}{d\varepsilon}\mathrm{d}\varepsilon$$

At each electron substep, MCNP/MCNPX uses $\sigma(\varepsilon_c)$ to determine randomly whether knock-on electrons will be generated. If so, the distribution of $\sigma(\varepsilon_c)$ will be used to sample the energy of each secondary electron. Once an energy has been sampled, the angle between the primary direction and the direction of the newly generated secondary particle is determined by momentum conservation. This angular deflection is used for the subsequent transport of the secondary electron. However, neither the energy nor the direction of the primary electron is altered by the sampling of the secondary particle. On the average, both the energy loss and the angular deflection of the primary electron have been taken into account by the multiple scattering theories.

Note, the concept of knock-on electrons from heavy charged particles is valid, however is not implemented in MCNPX version 2.3.0.

5 Multiparticle Extensions and General Tracking

MCNPX has expanded the capability of MCNP4B to track 34 particles, although in version 2.3.0, not all are fully transported. Those which are not transported typically have very short halflives, and are decayed immediately upon production (these are marked by a * in the mean lifetime column of Table 5-1). Decay of secondary particles continues until a set of transportable particles is obtained. Table 5-1 lists all particles currently defined in MCNPX version 2.3.0. Particles will be transferred to the "transportable" category in future versions as appropriate models of interaction physics are obtained.

Obviously, MCNPX has only one character to designate particle symbols, therefore we had to resort to symbols after the regular alphabet ran out. Output tables in the MCNPX OUTP file have been extended to support the additional tracked particles in a straightforward manner.

The list of particle properties, as well as decay branching ratios for non-tracked particles is derived from the *1998 Review of Particle Physics* (PDG98). The publication of the *Review of Particle Physics* is supported by the US Department of Energy, the US National Science Foundation, the European Laboratory for Particle Physics (CERN), by implementing arrangement between the government of Japan and the United States on cooperative research and development; and by the Italian National Institute of Nuclear Physics (INFN). It represents the current standard of international agreement on particle physics properties.

Table 5-1. Particles in MCNPX

IPT	Name of Particle	Symbol	Mass (MeV)	Low Kinetic Energy Cutoff (MeV)	Mean Lifetime (seconds) (* - decayed on production)
Original MCNP Particles					
1	neutron (n)	n	939.56563	0.0	887.0
1	anti-neutron (n)	n	939.56563	0.0	887.0
2	photon (γ)	p	0.0	0.001	huge
3	electron (e^-)	e	0.511008	0.001	huge
3	positron (e^+)	e	0.511008	0.001	huge
Leptons					
4	muon$^-$ (μ^-)	| ('pipe' symbol)	105.658389	0.11261	2.19703 x 10^{-6}

Table 5-1. Particles in MCNPX

IPT	Name of Particle	Symbol	Mass (MeV)	Low Kinetic Energy Cutoff (MeV)	Mean Lifetime (seconds) (* - decayed on production)
4	anti-muon$^-$ (μ^+)	|	105.658389	0.11261	2.19703 x 10^{-6}
5	tau$^-$ (τ^-)	*	1777.1	1.894	2.92 x 10^{-5} *
6	electron neutrino (ν_e)	u	0.0	0.0	huge
6	anti-electron neutrino	u	0.0	0.0	huge
7	muon neutrino (ν_m)	v	0.0	0.0	huge *
8	tau neutrino (ν_t)	w	0.0	0.0	huge *
Baryons					
9	proton (p)	h	938.27231	1.0	huge
9	anti-proton (p)	h	938.27231	1.0	huge
10	lambda^0 (Λ^0)	l (lower case L)	1115.684	1.0	2.632 x 10^{-2} *
11	sigma$^+$ (Σ^+)	+	1189.37	1.2676	7.99 x 10^{-3} *
12	sigma$^-$ (Σ^-)	-	1197.436	1.2676	1.479 x 10^{-2} *
13	cascade^0 (Ξ^0)	x	1314.9	1.0	2.9 x 10^{-2} *
14	cascade$^-$ (Ξ^-)	y	1321.32	1.4082	1.639 x 10^{-2} *
15	omega$^-$ (Ω^-)	o	1672.45	1.7825	8.22 x 10^{-3} *
16	lambda$_c{}^+$ ($\Lambda_c{}^+$)	c	2285.0	2.4353	2.06 x 10^{-5} *
17	cascade$_c{}^+$ ($\Xi_c{}^+$)	!	2465.1	2.6273	3.5 x 10^{-5} *
18	cascade$_c{}^0$ ($\Xi_c{}^0$)	?	2470.3	1.0	9.8 x 10^{-6} *
19	lambda$_b{}^0$ ($\Lambda_b{}^0$)	r	5641	1.0	1.07 x 10^{-4} *
Mesons					
20	pion$^+$ (π^+)	\	139.56995	0.14875	2.6033 x 10^{-8}
20	pion$^-$ (π^-)	\	139.56995	0.14875	2.6033 x 10^{-8}

Table 5-1. Particles in MCNPX

IPT	Name of Particle	Symbol	Mass (MeV)	Low Kinetic Energy Cutoff (MeV)	Mean Lifetime (seconds) (* - decayed on production)
21	neutral pion (π^0)	z	134.9764	0.0	8.4×10^{-17}
22	kaon$^+$ (K^+)	k	493.677	0.52614	1.2386×10^{-8}
22	kaon$^-$ (K^-)	k	493.677	0.52614	1.2386×10^{-8}
23	K_0 short	%	497.672	0.000001	0.8927×10^{-10}
24	K_0 long	^	497.672	0.000001	5.17×10^{-8}
25	D^+	g	1869.3	1.9923	1.05×10^{-4} *
26	D^0	d	1864.5	1.0	4.15×10^{-5} *
27	D_s^+	f	1968.5	2.098	4.67×10^{-5} *
28	B^+	j	5278.7	5.626	1.54×10^{-4} *
29	B^0	b	5279.0	1.0	1.5×10^{-4} *
30	B_s^0	q	5375.	1.0	1.34×10^{-4} *
Light Ions					
31	deuteron	d	1875.627	2.0	huge
32	triton	t	2808.951	3.0	12.3 years
33	Helium-3	s	2808.421	3.0	huge
34	Helium-4 (α)	a	3727.418	4.0	huge

Particle tracking between interactions involves several physics considerations which are described below. Atomic electron interactions will cause a charged particle to lose energy along its track length (ionization). Certain modifications to this energy loss are determined by “energy straggling” theory. Multiple scattering of charged particles is also implemented. Note that there is currently no “delta ray" production of knock-on electrons for charged heavy particles now in MCNPX version 2.3.0, although it is present for electrons.

No option for electromagnetic field tracking is currently implemented in MCNPX. Attempts are currently underway to develop this capability, which will be fully implemented in a future version of the code (FAV99).

5.1 Reaction Probability Calculation

Interaction physics in MCNPX is determined in two ways; through table-based data, and through on-line calculation with physics models. The physics models are used wherever the lower-energy tabular data are missing.

MCNPX version 2.3.0 can be used with any of the existing libraries now available for use with the MCNP4B code. These can be obtained through the RSICC facility at Oak Ridge National Laboratory, or through the NEA outside the United States. One set of libraries, however, is distributed directly with MCNPX; the new LA150 compendium (see Section 4.3.1).

In the physics module energy regime, the time tracking is governed by several cutoffs. The actual interaction chosen is the minimum in time of the following:

- Particle decay time (see Table 5-1, last column)
- Time to the next interaction as determined by the computed cross section
- Low energy cutoff (see Table 5-1, fifth column) Note that minimum energy cutoffs may be set by the user to .001 MeV for most particles. Neutrons, neutral pions and neutrinos are an exception, where a 0.0 cutoff can be set. However, unless there is tabular data or a specially implemented low energy physics model, no interactions of these particles will occur between below the minimum recommended in Table 5-1.
- User-specified time cutoff

5.2 Collisional Stopping Power for Heavy Charged Particles

An improved collisional energy-loss model has been added to MCNPX, by modifying the stopping-power module of LCS in several ways. The ionization potentials have been enhanced to the values and interpolation procedures recommended in ICRU Report 37 (ICR84), bringing the model into closer ICRU compliance. The density effect correction now uses the parameterization of Sternheimer and Peierls (STE71). Additional improvements to the density effect calculation recommended in ICRU Report 37 will be incorporated in a future release.

For high-energy protons and other light charged projectiles, the approximate SPAR model (ARM73) has been replaced with a full implementation of the maximum kinetic energy transfer. For intermediate energies, the shell corrections to the stopping power have been adapted from Janni (JAN82). Finally, a continuous transition in the stopping power between the ranges 1.31 MeV/AMU (Atomic Mass Unit) for the high-energy model, and 5.24 MeV/AMU (the low energy SPAR model) is achieved with a linear interpolation between the two models.

These new procedures provide a small but significant improvement over LAHET practice above 1 MeV/AMU, while offering a smoother transition to the low energy model. A more detailed discussion can be found in PRA98b.

Due to nonlinearities in the ionization implementation for heavy charged particles, we do not recommend that the MCNPX user define more than one density for the same material. Different **Mn** cards should be included for different densities (see Section 6.1.6).

5.3 Energy Straggling for Heavy Charged Particles

MCNPX, like MCNP4B, uses a sophisticated implementation of the Landau theory for electrons (see Section 4.3.3.2). For heavy charged particles, the assumptions of the Landau theory break down, and the more complex Vavilov theory (VAV57) must be used. At low energies and large step sizes, the Vavilov distribution approaches a Gaussian. At very high energies, or small step sizes (and for electrons in almost all circumstances), the Vavilov distribution approaches a Landau distribution. The module implemented in MCNPX to represent the Vavilov model does attempt to account for the Gaussian and Landau limits, when step sizes and energies are appropriate for heavy charged particles. This will be incorporated in future versions of the code.

An improved detailed logic for the use of the Vavilov straggling model for heavy charged particles is available (and is now the default) in Version 2.3.0. Previously, the Vavilov model was used to establish a straggled energy-loss rate closely tied to the step-lengths of the major energy steps of the transport. The smaller angular substeps and partial substeps to boundaries or to potential interactions relied on a simple interpolation for an estimate of energy loss. In addition, departure from the initial energy group during the substep was ignored. The new logic applies the Vavilov algorithm to each substep and to each partial substep, and makes a better estimate of the continuous-slowing-down energy loss (mean energy loss) across energy-group boundaries. The new treatment leads to considerably improved results in a variety of physically interesting calculations, such as the range of heavy charged particles. A full description of the algorithm and some examples of the results can be found in a recent Los Alamos Research Note [PRA00a].

5.4 Multiple Scattering for Heavy Charged Particles

The full Goudsmit-Saunderson model of multiple scattering for electrons as implemented in MCNP4B/MCNPX was described in Section 4.3.3.2.

In MCNPX version 2.3.0, a small-angle Coulomb scattering treatment has been implemented for heavy charged particles. We use a Gaussian model based on a theory presented by Rossi. In the original theory, both angular deflections and small spatial displacements were accounted for. Since the complex geometric system of MCNPX does not yet accommodate transverse displacements in charged-particle substeps, we use only the part of the theory that addresses the angular deflection. In several test cases, this slight approximation has been found to have negligible effect on the results.

6 MCNPX Input Files

Standard MCNP input cards are all accepted in MCNPX, however additional card options are now available to take advantage of the multiparticle capabilities. Modifications to standard MCNP inputs are described in Section 6.1. Section 6.2 describes new cards added to control the Bertini, ISABEL and CEM physics options, which are used when table-based data are not available. Use of new high-energy, proton, and photonuclear data library capabilities has already been described in Section 4.3.

Accelerator simulation applications have a need for specialized source input to describe an incident particle beam. Usually this takes the form of a directed beam of particles, monoenergetic, with a transverse gaussian profile. To facilitate this, a new source option has been added to MCNPX and is described in Section 6.3.

6.1 MCNP Card Modifications and Additions

6.1.1 Problem Type Card

MODE

The **MODE** card can now take any argument listed in the “Symbol" column of Table 5-1, in any order. It must list all particles that will be transported. If a particle is designated, the anti-particle will also be transported. For example, MODE n h | e will transport neutrons and anti-neutrons, protons and anti-protons, μ^+ and μ^-, electrons and positrons.

6.1.2 Geometry Cards

VOL AREA U TRCL LAT FILL TR

No modifications have been made to any cell or surface card.

6.1.3 Variance Reduction Cards

IMP ESPLT PWT EXT VECT FCL WWE WWN WWP WWG WWGE PDn DXC BBREM

Any card with a particle designator can accept any particle symbol from Table 5-1. A new type of biasing (secondary particle biasing) has been added and is described in Section 7.1.

Note: Detector variance reduction techniques will not work outside library energy limits. Detector variance reduction techniques will also not work for charged particles.

6.1.4 Source Specification Cards

SDEF SIn SPn SBn DSn SCn SSW SSR KCODE KSRC

All source capabilities of MCNP are intact, and additional features have been added to describe typical accelerator beams (see Section 6.3).

The argument **PAR** can be set to any IPT value in Table 5-1. Since particles and antiparticles have the same IPT values, an antiparticle source is designated with a minus sign. For example, **PAR=-9** will generate antiprotons in an **SDEF** card.

Note: In MCNPX version 2.3.0, one cannot use positrons as a source (**PAR=-3**). This will be implemented in a near-term future version. As in MCNP, only one source particle can be designated at any one time.

When **PAR** is absent, the source particle generated depends on the arguments of the **MODE** card. The general rule in MCNP is that the particle with the lowest IPT value (see Table 5-1) specified on the MODE card will be the source particle. Thus **MODE n h /** would result in a neutron source.

A modification has been made to the built-in function for source probability, F=-41. The gaussian distribution in time has been converted to a gaussian distribution in space in order to model accelerator particle beams. This modification is discussed in Section 6.3.

6.1.5 Tally Specification Cards

F1:p F2:p F4:p F5a:p F6:p F7:n F8:p

Any card with a particle designator can accept all new particle types. The **F6** energy deposition options have been changed to accommodate the larger particle list. A new **+F6** tally has been added to tally energy deposition from individual particle types (see Section 8.3). New Mesh Tally and Radiography tally capabilities have been added (See Sections 8.1 and 8.2)

6.1.6 Material Specification Cards

Mm DRXS TOTNU NONU AWTAB XSn VOID PIKMT MGOPT

No changes have been made to any material specification cards for neutron problems.

We have made the designation of materials with more than one density a fatal error, due to non-linear density scaling effects for charged particle transport. We recommend defining materials with more than one density should this case be encountered. The fatal error can be overridden by setting the 19th entry of the **DBCN** card to a non-zero value. This will disable all fatal errors, so the user should use extreme caution when doing this.

Additional cards are needed when specifying photonuclear libraries. Since there are a limited set of libraries available, there may not be a photonuclear table corresponding to the neutron, proton, electron or photon ZAID's on the Mm card. A new card has been developed to instruct the code what to do in such cases. [WHI00].

MPNn **PNZA$_1$** **PNZA$_2$** **...** **PNZA$_{\#Mn\ Pairs}$**

For material n, one can enter the isotope description from which to get photonuclear data for all elements listed on the **Mn** card. A Zero entry for PNZA will turn off photonuclear interactions for that particular element.

6.1.7 Energy and Thermal Treatment Cards

PHYS TMP THTME MTm

A **PHYS** card may be specified for any particle type, and we recommend that they be included for all particles on the **MODE** card.

Charged and Neutral Particles except Photons:

The first entry on the **PHYS** card, is the maximum energy for the specified particle. Note that the default **EMAX** can be quite low, and failing to reset this for high energy problems will result in code termination because particle energies exceed **EMAX**. The code will note the largest **EMAX** from all the specified **PHYS** cards in the problem. If a tracked particle does not have a **PHYS** card, its **EMAX** will be set to this largest value. If no **PHYS** cards are included in the problem, **EMAX** is set to 100 MeV for all particles.

A third argument has been added to the **PHYS:n and PHYS: h** cards to accommodate the extended 150 MeV neutron and proton libraries. Set the **CUT_N** or **CUT_H** value to the maximum energy to which table-based data will be used for neutrons (MCNPX version 2.1.5 and later) and for protons (MCNPX version 2.3.0).

The **CUT** parameter must be used with caution. MCNPX 2.3.0 cannot yet combine libraries with different upper energy limits, however it is not a fatal error to call for a combination of such libraries. Several examples can illustrate the potential problem (20 and 150 MeV libraries are our most commonly available tables, however the user should be aware that other upper limits might be present).

- if **CUT** is set to 20.0, and all libraries have upper energies of 20.0, then libraries will be used to 20 MeV, and physics models above that energy.
- if **CUT** is set to 20.0, and all libraries have upper energies of 150.0, then libraries will be used to 20 MeV, and physics models above that energy.
- if **CUT** is set to 150.0 and any library has an upper energy of 20.0, then the code will use the cross section values found at 20 MeV in that library from 20 to 150 MeV. No

attempt at extrapolation of the 20 MeV value to a value at 150 MeV will be made, since there is currently no means determine the 150 MeV cross section value.

Note that one can specific different values for **CUT_N** and **CUT_H**. For example, specifying **CUT_H = 0** will tell the code not to use any proton libraries, only physics models.

```
PHYS:n          EMAX    EMCNF  CUT_N
PHYS:h          EMAX    EMCNF  CUT_H        j         ISTRAG
PHYS:e          EMAX IDES IPHOT IBAD ISTRG BNUM XNUM RNOK ENUM
                (see MCNP4B manual for electron definitions)
PHYS:(all other charged particles)
                EMAX    j          j            j         ISTRAG
```

Table 6-1. Setting upper limits for neutron & proton tabular data

Keyword	Description
EMAX	Upper limit for neutron or proton energy (MeV)
EMCNF	Energy boundary (MeV) above which neutrons are treated with implicit capture and below which they are treated with analog capture. This variable is not read in for protons.
CUT_N **CUT_H**	Energy (MeV) below which table based data are used, and above which physics modules are used. Neutron default is 20.0 MeV, proton default is 0.0 MeV.
unused	
ISTRG	0 = improved approach to Vavilov straggling (default) 1 = continuous slowing down approximation -1 = old Vavilov treatment from 2.1.5 ISTRG was placed in the 5th position of the PHYS card for heavy charged particles in order to be consistent with the corresponding entry on a PHYS:e card. ISTRG is not used for neutrons

Photons:

After the maximum energies for all other particles have been set, photons are considered. If photons are being transported, a photon maximum energy is set as the lowest of the set of maximum energies found among photon tables in the problem. If electrons are being transported, or only photons but with consideration of secondary electron (thick-target bremsstrahlung) then the photon maximum energy is adjusted to be no higher than the electron maximum energy.

In order to turn on photonuclear interactions, a fourth entry (**PNINT**) has been added to the **PHYS** card when used with the '**p**' designator [WHI00]:

PHYS:p EMCPF IDES NOCOH PNINT

Table 6-2. Turning on Photonuclear Interactions

Keyword	Description
EMCPF	Upper energy limit (in MeV) for detailed photon physics treatment
IDES	0 = photons will produce electrons in MODE E problems or bremsstrahlung photons with the thick target bremsstrahlung model 1 = photons will not produce electrons as above
NOCOH	0 = coherent scattering occurs 1 = coherent scattering will not occur
PNINT	1 = Analog photonuclear interactions turned on 0 = Photonuclear interactions turned off (default) -1 = Biased phtonuclear interactions turned on

No changes have been made to the **TMP**, **THTME** or **MTm** cards.

6.1.8 Problem Cutoffs Cards

CUT ELPT NPS CTME

The **CUT** and **ELPT** cards can now designate any particle symbol.

NPS can now have two arguments related to the radiography tally capability. These are discussed in Section 8.2.2.

Note: A default set of low energy cutoffs is in place (see Table 5-1). Energies for particles other than neutrons, neutrinos and photons can be set to a minimum of 1 keV (the exceptions can be set to 0.0 MeV). However, no interaction physics is present between 1 keV and the default minimum.

Note: Care must be taken for non-standard code terminations when using the **HTAPE3X** program. Normalization may not be what NPS indicates. See Section 8.5 for details.

6.1.9 Peripheral Cards

PRDMP LOST DBCN FILES PRINT MPLOT PTRAC PERT

No changes have been made in peripheral cards.

6.1.10 New Cards Specific to MCNPX

The following cards are new to MCNPX. Detailed explanations can be found in the association manual sections.

LCA LCB LEA LEB
These cards control physics parameters for the BERTINI, ISABEL, CEM and FLUKA options. See Section 6.2

HISTP
This card will turn on the production of the LAHET-compatible HISTP file. See Section 8.5

SPABI
Secondary particle biasing variance reduction. See Section 7.1.

TMESH (R/C/S)MESHn CORAn CORBn CORCn ENDMD ERGSH MSHMF
Mesh Tally Cards. See section 8.1.

FIn PIn FSn Cn TI(R/C)n TIR TIC NOTRN TALNP
Radiography tally cards. See section 8.2.

6.2 Physics Module Options

Four new MCNPX input cards have been defined to allow the user control of physics options. A summary of the cards follows. The options controlling the Bertini and ISABEL physics modules are taken from the User Guide to LCS (PRA89). The user is referred to that document for further information.

CEM allows neutrons and protons up to 5 GeV and pions up to 2.5 Gev to initiate nuclear reactions. Valid targets are nuclei with a charge number greater than 5, and a mass number greater than 11. The light nuclei are passed to the Bertini/ISABEL models that use the Fermi-Breakup model in this regime. CEM consists of an intranuclear cascade model, followed by a pre-equilibrium model and an evaporation model. Possible fission events are initiated in the equilibrium stage for compound nuclei with a charge number greater than 70. The fragmentation of the fission event is handled by modules from the RAL fission model. Fission fragments undergo an evaporation stage that depends on their excitation energy. After evaporation a de-excitation of the residual nuclei follows, generating gammas using the PHT data.

Future developments of MCNPX will allow greater freedom in the selection of physics options (INC, pre-equilibrium, evaporation, fission, etc.) so the user may compare the effect of varying one parameter at a time. In version 2.3.0, CEM is still relatively self-contained.

All of the input values on the four cards have defaults, which will be taken in the absence of the cards, or with the use of the MCNP-style **J** input option.

LCA IELAS IPREQ IEXISA ICHOIC JCOUL NEXITE NPIDK NOACT ICEM

LCA is used to select the Bertini, ISABEL or CEM models, as well as set certain parameters used in Bertini and ISABEL. CEM is a self-contained package with no internal options presently defined.

Table 6-3. LCA Keyword Descriptions

Keyword	Description
IELAS	0 = No nucleon elastic scattering 1 = elastic scattering for neutrons only 2 = elastic scattering for neutrons and protons (default)
IPREQ	0 = No pre-equilibrium model will be used 1 = Use pre-equilibrium model after intranuclear cascade (default) 2 = Use **IPREQ**=1 and **IPREQ**=3 randomly, with an energy-dependent probability that goes to **IPREQ**=3 at low energies and to IPREQ=1 at high incident energies 3 = Use pre-equilibrium model instead of the intranuclear cascade. **Note**: 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
IEXISA	0 = Do not use ISABEL intranuclear cascade model for any particle 1 = Use Bertini model for nucleons and pions, with ISABEL model for other particle types (default) 2 = Use ISABEL model for all incident particle types. **Note**: The ISABEL INC model requires a much greater execution time. In addition, incident particle energies should be less than 1 GeV, or 1 GeV per nucleon for composite particles (although it may execute at higher energies)

Table 6-3. LCA Keyword Descriptions (Continued)

Keyword	Description
ICHOIC	4 integers (ijkl) which control ISABEL INC Model (default = 0023) i = 0 Use partial Pauli blocking i = 1 Use total Pauli blocking i = -2 No Pauli blocking (not recommended) j = 0 No interaction between particles already excited above the Fermi Sea j > 0 Number of time steps to elapse between such "CAS-CAS" interactions k = 0 Meyer's density prescription with 8 steps k = 1 Original (isobar) density prescription with 8 steps k = 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 k = 3 The same as k=0 but using the larger nuclear radius of the Bertini model k = 4 The same as k=1 but using the larger nuclear radius of the Bertini model k = 5 The same as k=2 but using the larger nuclear radius of the Bertini model l = 1 Reflection and refraction at the nuclear surface, but no escape cutoff for isobars l = 2 Reflection and refraction at the nuclear surface, with escape cutoff for isobars l = 3 No reflection or refraction, with escape cutoff for isobars l = 4 The same as l=1 but using a 25 MeV potential well for pions l = 5 The same as l=2 but using a 25 MeV potential well for pions l = 6 The same as l=2 but using a 25 MeV potential well for pions **Note**: Not all the options for the ISABEL INC model have been thoroughly debugged.
JCOUL	1 = Use Coulomb barrier on incident charged-particle interactions (default) 0 = No Coulomb barrier for incident charged particles
NEXITE	1 = Subtract nuclear recoil energy to obtain nuclear excitation energy (default) 2 = Do not subtract nuclear recoil energy
NPIDK	1 = Force π^- to terminate by decay at the pion cutoff energy 0 = Force π^- to interact by nuclear capture (INC) when cutoff is reached (default) **Note**: The capture probability for any isotope in a material is proportional to the product of the number fraction and the charge of the isotope. However, capture on ^{1}H leads to decay rather than interaction.

Table 6-3. LCA Keyword Descriptions (Continued)

Keyword	Description
NOACT	**Note**: The use of the **NOACT** option other than the default is intended as a diagnostic tool, allowing other processes to be more easily observed. [PRA99] 2 = Attenuation mode (transport primary source particles without nonelastic reactions). 1 = Do not turn off nonelastic reactions (default) 0 = Turn off all nonelastic reactions. -1 = Compute nuclear interactions of source particles only - transport and slowing-down are turned off. This option is for use in computing double-differential particle production cross sections with the XSEX code (See Appendix C).
ICEM	0 = Use the Bertini or ISABEL model (determined by the **IEXISA** parameter) (default) 1 = Use the CEM model

LCB FLENB1 BLENB2 FLENB3 FLENB4 FLENB5 FLENB6 CTOFE FLIM0

LCB controls which physics module is used for particle interactions depending on the kinetic energy of the particle.

Table 6-4. LCB Keyword Descriptions

Keyword	Description
FLENB1	Kinetic Energy (Default = 3500 MeV) For nucleons the Bertini INC model will be used below this value
FLENB2	Kinetic Energy (Default = 3500 MeV) For nucleons the FLUKA high-energy generator will be used above this value. **Note**: The probability for selecting the interaction model is interpolated linearly between **FLENB1** and **FLBEN2**. **Note**: The version of FLUKA used in MCNPX version 2.3.0 should not be used below 500 MeV/;c (momentum). **Note**: For nucleons, the Bertini model switches to a scaling procedure above 3.495 GeV, wherein results are scaled from an interaction at 3.495 GeV. Although both models will execute to arbitrarily high energies, a plausible upper limit for the Bertini scaling law is 10 GeV.
FLENB3	Kinetic Energy (Default = 2500 MeV) For pions the Bertini INC model will be used below this value.
FLENB4	Kinetic Energy (Default = 2500 MeV) For pions the FLUKA high-energy generator will be used above this value. See **Notes** under **FLENB2**.
FLENB5	Kinetic Energy (Default = 800 MeV) For nucleons the ISABEL INC model will be used below this value.
FLENB6	Kinetic Energy (Default = 800 MeV) For nucleons an appropriate model will be used above this value. for **IEXISA** = 2 it applies to all particle types. for **IEXISA** = 1 it applies to all particles except nucleons and pions. for **IEXISA** = 0 it is immaterial See the example following this table for further explanation.

Table 6-4. LCB Keyword Descriptions (Continued)

Keyword	Description
CTOFE	The cutoff kinetic energy (MeV) for particle escape during the INC *when using the Bertini model*. The cutoff energy prevents low energy nucleons from escaping the nucleus during the INC; for protons, the actual cutoff is the maximum of CTOFE and a Coulomb barrier. **CTOFE** >= 0 **CTOFE** will be used as the cutoff energy. **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 (CTOFE = -1.0). For the ISABEL INC, the randomized cutoff energy is always used.
FLIM0	The maximum correction allowed for mass-energy balancing in the cascade stage, used with **NOBAL**=1 and **NOBAL**=3. **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 re sampled if the correction exceeds **FLIM0**. **FLIM0** = 0 No correction will be attempted and a cascade will be re-sampled if a negative excitation is produced. **FLIM0** < 0 (default = -1.0) 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.

As an example consider:

```
LCB       3000 3000 2000 2000 1000 1000
```

For **IEXISAQ** = 1, the default, nucleons will switch to the BERTINI model from the FLUKA model below 3 GeV, and Pions would switch below 2 GeV. Kaons and anti-nucleons would switch to the ISABEL model from the FLUKA model below 1 GeV. (Ions use only the ISABEL model, and muons have no nuclear interactions.

For **IEXISA**=2, nucleons and pions would also switch to the ISABEL model below 1 GeV. Note that the nominal upper energy limit for the ISABEL model is about 1 GeV/nucleon; it may actually execute at higher energies without crashing, but with diminished validity.

LEA IPHT ICC NOBALC NOBALE IFBRK ILVDEN IEVAP NOFIS

LEA controls evaporation, fermi-breakup, level density parameters and fission models. All of these are external to the particular intranuclear cascade/pre-equilibrium model chosen (Bertini, ISABEL, or CEM), and may be used with any of these choices.

Table 6-5. LEA Keyword Descriptions

Keyword	Description
IPHT	0 = Do not generate photons in the evaporation stage. 1 = Generate de-excitation photons (default).
ICC	Defines the level of physics to be applied for the PHT physics. 0= The continuum model 1= Troubetzkoy (E1) model 2 = Intermediate model (hybrid between 1 and 2) 3 = The spin-dependent model 4 = The full model with experimental branching ratios (default)
NOBALC	0 = Use mass-energy balancing in the cascade phase. 1 = Turn off mass-energy balancing in the cascade phase (default). **Note**: A forced energy balance may distort the intent of any intranuclear cascade model. Energy balancing for the INC is controlled by the input parameter **FLIM0**.
NOBALE	0 = Use mass-energy balancing in the evaporation stage (default). 1 = Turn off mass-energy balancing in the evaporation stage.
IFBRK	1 = Fermi breakup model for A ≤ 13 and for 14 ≤ A ≤ 20 with excitation below 44 MeV (default). 0 = Use Fermi breakup model only for A ≤ 5.
ILVDEN	-1 = Use original HETC level density formulation. See the **LEB** card for details on parameter inputs. 0 = Use Gilbert-Cameron-Cook-Ignatyuk level density model (PRA88) (default). 1 = Use the Julich level density parameterization as a function of mass number (CLO83).
IEVAP	0 = The RAL evaporation-fission model (ATC80) will be used (default). 1 = The ORNL evaporation-fission model (BAR81) will be used. **Note**: The ORNL model allows fission only for isotopes with Z≥91.
NOFIS	1 = Allow fission (default) 0 = Suppress fission

LEB YZERE BZERE YZERO BZERO

This card controls level density input options for the original HETC implementation.

Table 6-6. LEB Keyword Descriptions

Keyword	Description
YZERE	The Y0 parameter in the level density formula for Z ≤ 70 The default is 1.5; zero or negative is an error condition. For target nuclei with Z ≤ 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 ≥ 71, the **BZERO** and **YZERO** parameters are used to compute level densities for the target nucleus and fission fragments. **Note**: Applies only for **ILVDEN** = -1.
BZERE	The B0 parameter level density formula for Z ≤ 70. The default is 8.0; zero or negative is an error condition (see YZERE above). **Note**: Applies only for **ILVDEN** = -1.
YZERO	The Y0 parameter in the level density formula for Z ≥ 71 and all fission fragments. The default is 1.5. Zero and negative values are an error condition (see YZERE above). **Note**: Applies only for **ILVDEN** = -1.
BZERO	The B0 parameter in the level density formula for Z ≥ 71 and all fission fragments. The default is 10.0 for IEVAP = 0 and is also 10.0 for IEVAP = 1. Zero and negative values are an error condition (see YZERE above). **Note**: Applies only for **ILVDEN** = -1.

6.3 Extended Source Options

The extended source option has been adapted from similar capabilities in the LAHET Code System as described in PRA99.

Two features have been added in MCNPX to the MCNP general source routines. The first is a simple modification that permits the use of an **f=-41** Gaussian probability distribution for the X, Y or Z positional parameters on the SDEF card. In MCNP, the **-41** option has been used for a time gaussian distribution; in MCNPX the fatal error for specifying the spatial option has been removed. This allows creation of a Gaussian beam profile, however the user should keep in mind that many realistic accelerator beams are only approximately Gaussian, and normally have enhanced tails due to particle interactions in the upstream accelerator. If needed, such fine detail must be specified with standard MCNP source specification methodology.

An additional feature has been added through the specification of a general transformation on the SDEF card in one of two forms; **TR = n** or **TR = Dn**. In either case a general transformation is applied to a source particle *after* its coordinates and direction cosines have been determined using the other parameters on the **SDEF** card. Particle coordinates are modified by both rotation and translation; direction cosines are modified by rotation only. This allows the user to rotate the direction of the beam or move the entire beam of particles in space. The **TR=Dn** card is particularly powerful, since it allows the specification of more than one beam at a time.

An example of specifying a Gaussian beam is given below and may be modified at the user's need:

```
Title
c Cell cards
...
ccc          0       -nnn            ! cookie cutter cell

c Surface Cards
...
nnn          SQ     a^-1    b^-2    0 0 0 0 -c^2 0 0 0   ! cookie cutter surface

c Control Cards
SDEF         DIR=1   VEC=0 0 1   X=D1   Y=D2   Z=0   CCC=ccc   TR=n
SP1          -41     f_x     0
SP2          -41     f_y     0
TRn          x_0 y_0 z_0   cosφ  -sinφ   0   sinφ   cosφ   0     0 0 1
```

The **SDEF** card sets up an initial beam of particles travelling along the Z axis (**DIR=1**, **VEC=0 0 1**). Information on the x and y coordinates of particle position is detailed in the two **SP** cards (**X=D1**, **Y=D2**, indicating that the code must look for distributions 1 and 2, here given by source probability distributions **SP1** and **SP2**). The z coordinate is left unchanged (**Z=0**).

There is no **PAR** option in this example, therefore the particle generated by this source will be the one with the lowest IPT number in Table 5-1 (neutron).

The SP cards have three entries. The first entry is **-41**, which indicates sampling from a built-in gaussian distribution (note, the function -41 is a gaussian in time in MCNP. It has been modified for the purpose of MCNPX). It has the following density function:

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

The parameters a and b are the standard deviations of the Gaussian in x and y.

The second entry (f_x or f_y) on the SP cards is the full width half maximum (FWHM) of the Gaussian in either the x or y direction, and must be computed from a and b by the user as follows:

$$f_x = (8\ln 2)^{\frac{1}{2}}a = 2.35482a$$

$$f_y = (8\ln 2)^{\frac{1}{2}}b = 2.35482b$$

The third entry represents the centroid of the Gaussian in either the x or y direction. We recommend that the user input 0 here, and handle any transformations of the source with a TR card as described below. Using a non-zero value will interfere with the rejection function as specified by the “cookie cutter” option.

Note, that in Table 10 in the MCNPX output file, the definitions of a, b, and c are different from those discussed above, however fwhm will be the same as the 3rd entry on the SP cards. The parameter ‘a’ in Table 10 differs from the parameter ‘a’ above by a factor of the square root of 2. This is a legacy item from the conversion of the -41 function from time to space, and will be corrected in a future version.

The user generally does not want the beam Gaussian to extend infinitely in x and y, therefore a cookie cutter option has been included to keep the distribution to a reasonable size. **CCC=ccc** tells MCNPX to look at the card labeled **ccc** (**ccc** is a user-specified cell number) to define the cutoff volume. The first entry on the **ccc** card is **0**, which indicates a void cell. The second number, **-nnn** (**nnn** again is a user specified number), indicates a surface card within which to accept particles. In the example, this is a SQ surface, a 2-sheet hyperboloid is defined as follows:

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

Any particle generated within this cell is accepted; any outside of the cell is rejected. Any well-defined surface may be selected, and it is common to use a simple cylinder to represent the extent of a beampipe.

In this example, a source is generated in an (x', y') coordinate system with the distribution centered at the origin and the particles travelling in the z' direction. The particle coordinates can be modified to an (x,y) coordinate system by translation and rotation according to the following equations, where $0 \le \phi_L \le \pi$:

$$x = x'\sin\phi_L - y'\cos\phi_L + x_0$$

$$y = x'\cos\phi_L + y'\sin\phi_L + y_0$$

Thus the angle ϕ_L is the angle of rotation of the major axis of the source distribution from the positive y-direction in the laboratory coordinate system. If $\cos\phi_L = 0.0$ the angle is 90^o and the major axis lies along the x-axis. The **TRn** card in the above example implements this rotation matrix, however the user is warned that ϕ in the **TRn** card is equal to $\phi_L - \frac{\pi}{2}$.

Defining Multiple Beams

The opportunity to specify a probability distribution of transformations on the **SDEF** card is a new feature that goes beyond enabling the representation of LAHET beam sources. It allows the formation of multiple beams which differ only in orientation and intensity; a feature that may have applications in radiography, or in the distribution of point sources of arbitrary intensity.

The use of a distribution of transformations is invoked by specifying **TR=Dn** on the **SDEF** card. The cards **SI**, **SP** and optionally **SB** are used as specified for the **SSR** card on page 3-57 of the MCNP4B User's Guide.

SIn	L	$I_1 ... I_k$
SPn	option	$P_1 ... P_k$
SBn	option	$B_1 ... I_k$

The L option on the **SI** card is required; new input checking has been implemented to ensure this usage for both the **SDEF** and **SSR** applications. The "option" on the **SP** and **SB** cards may be blank, D or C. The values $I_1 ... I_k$ identify k transformations which must be supplied. The content of the SP and SB cards then follows the general MCNP rules.

The following example shows a case of three intersection Gaussian parallel beams, each defined with the parameters a=0.2cm, b=0.1cm and c=2 in the notation previously discussed. For each, the beam is normal to the plane of definition.

- Beam 1 is centered at (0,0,-2) with the major axis of the beam distribution along the x-axis, emitted in the +z direction, with relative intensity 1.
- Beam 2 is centered at (-2,0,0) with the major axis of the beam distribution along the y-axis, emitted in the +x direction, with relative intensity 2.
- Beam 3 is centered at (0,-2,0) with the major axis of the beam distribution along the line x=z, emitted in the +y direction, with relative intensity 3.

The card **SBn** is used to provide equal sampling from the three beams which is independent of the relative intensities. This example demonstrates most of the new features. The input cards are as follows:

```
Title
c Cell cards
...
999          0       -999    ! cookie cutter cell

c Surface Cards
...
999          SQ      25      100     0 0 0 0 -4  0 0 0   ! cookie cutter surface

c Control Cards
SDEF         DIR=1   VEC=0 0 1   X=D1    Y=D2    Z=0    CCC=999   TR=D3
SP1          -41     .470964     0
SP2          -41     .2358482    0
SI3          L 1 2 3
SP3          1 2 3
SB3          1 1 1
TR1          0 0 -2  1 0 0       0 1 0       0 0 1
TR2          -2 0 0  0 1 0       0 0 1       1 0 0
TR3          0 -2 0    .707 0.707        .707 0 -.707      0 1 0
```

7 New Variance Reduction Techniques

The high-energy cascade process generates numerous particles over a very broad range of energies (at Super Collider energies, 20 TeV + 20 TeV proton collisions, the average number of particles generated for a central collision is ~19,000!). This is a far different situation from what the typical low energy MCNP user is accustomed, and standard methods such as fixed cell importance biasing applied equally to all particles is not always the best solution. At a minimum, one should consider biasing in both spatial cells and energy groups, and the complexity of the problem leads one to consider semi-automatic schemes such as the weight window generator, DSA, etc. Special variance reduction techniques have also been developed in the industry to enhance the production of particles of interest. One example is Leading Particle biasing, where production of only the highest energy, most promptly produced particles is enhanced.

In addition, one cannot assume isotropy of particle emission at high energies, and the actual emission pattern varies over a wide range. This anisotropy causes problems in using detector techniques for neutral particles above library energies. Closely related to this is the fact that no adequate algorithm yet exists for charged-particle detectors.

MCNPX has an active program of improvement in high-energy and charged-particle variance reduction techniques, and features will be added in future versions as they are developed. MCNPX version 2.3.0 has currently implemented one special technique, Secondary Particle biasing, described in Section 7.1.

7.1 Secondary Particle Biasing

Secondary particle biasing has been introduced into the MCNPX code for two main reasons.

- It allows splitting of secondary particles from high-energy cascades in the energy range of interest.
- It allows the user to roulette the large number of particles in energy ranges that are of no interest to the problem.

This technique is especially useful in deep penetration problems starting with very high-energy particles where the very large number of low-energy secondary particles have little or no chance of contributing to the answer. On the other hand, one needs all of the high-energy particles that one can get.

MCNPX version 2.3.0 has been upgraded to allow the user to control the numbers of secondary particles as a function of energy and primary particle interaction. To this end, a new card has been added to the INP file as shown below:

SPABI:p xxx... E1 S1 E2 S2 ...

Table 7-1. Secondary Particle-Biasing Argument Descriptions

Argument	Description
p	Secondary Particle Type (see Table 5-1)
xxx...	List of primary particles to be considered. • For example, **nphe** represents reactions of neutrons, photons, protons, and electrons. No spaces are allowed. • If all particles are to be considered, the entry should be **all**.
En	Upper energy bin limit. The lower bin limit is considered to be zero.
Sn	Use Splitting if **Sn** > 1 Splitting Use Roulette if 0<= **Sn**<=1

As many **SPABI** cards as needed can be used to cover any number of secondary particle types and there is no limit on the number of **En Sn** pairs.

Every time an interaction takes place in MCNPX which results in secondary particles generation, the code checks to see if secondary particle biasing is turned on. If so, the particle causing the interaction is compared with the list of primary particles on the **SPABI** card to see if these secondary particles are to be considered or not. If the primary particle is in the list, the secondary particle energy is used to determine the energy bin and subsequent splitting or roulette to be played before the particles are banked. An adjustment is then made to the number of particles resulting from this type interaction scored in the summary tables.

It should be noted that all of the split particles coming out of the bank are identical. Therefore, if there is little or no scattering media between the banked particles and the tallies, this type of splitting could be a total waste of time. Roulette, on the other hand, eliminates the need to transport and tally a large number of insignificant particle tallies. As with any splitting or roulette game, the weights of the banked particles have to be adjusted to make the tallies correct. In order to insure that the weight cutoff game does not have an adverse effect on the particles because of this type of weight reduction, a splitting/roulette factor is generated and banked with the particle. When the weight cutoff game is played, this factor is used to adjust the weight much in the same way as the adjustment made for cell splitting and roulette. This factor could probably be used to correct a weight cutoff problem encountered with the energy splitting option currently in the code.

8 New and Improved Tallies and Data Analysis

No fundamental changes have been made to the format of any output table as currently found in MCNP4b, however additional lines have been added for information on the new particles. These should be obvious, and will not be described in detail.

MCNPX includes several new tally capabilities (section 8.1, 8.2 and 8.3), as well as modifications to the Energy Deposition scoring capabilities (section 8.4). In addition, the MCNPX distribution includes the HTAPE3X code for backward compatibility with the LAHET Code System (section 8.5).

The new 'visual' tallies (Mesh and Radiography tallies) are provided with an interpretation program, **gridconv** (sections 8.1.2 and 8.2.4). This stand-alone program converts the output of the tallies into a format consistent with several currently available graphics packages. In MCNPX 2.3.0, **gridconv** will also convert the results of any tally contained in a MCTAL file. This capability is described in the general **gridconv** discussion of section 8.1.2.

Parallel processing is not yet implemented in MCNPX; this is a major development which will be integrated into new data structures to be added in MCNPX version 3.0. We fully realize that applications in high energy regimes are computationally intensive, and it has been long established practice to run Monte Carlo codes on many machines, adding the final results together. Notes for the user on this practice are given in section 8.6

8.1 The Mesh Tally

The technique which has become known as the "Mesh Tally" has become very widely used in many applications. The development of this method grew out of research with codes such as LCS, GEANT, FLUKA, CALOR, and MARS at the Superconducting Super Collider in 1993. Some form of this method is currently in standard use in most high-energy Monte Carlo codes.

The Mesh Tally is a method of graphically displaying particle flux, dose, or other quantities on a rectangular, cylindrical, or spherical grid overlaid on top of the standard problem geometry. Particles are tracked through the independent mesh as part of the regular transport problem, and the contents of each mesh cell written to a file at the end of the problem. This file can be converted into a number of standard formats suitable for reading by various graphical analysis packages. The conversion program, **gridconv,** is supplied as part of the overall MCNPX package (section 8.1.2). An example of a mesh tally plot is shown in Fig.

8-1. This represents a plan view of neutron fluence in a spallation target system. Analysis of this data is limited only by the capabilities of the graphical program being used.

8.1.1 Setting up the Mesh in the INP File

A mesh tally is defined by several cards which are described below. All of the control cards for mesh tallies must be in a block preceded by a card containing the word **tmesh** in the first five columns, and terminated by a card containing the word **endmd** in the first five columns. For each mesh tally card, the following set of cards must be present which give details on the mesh characteristics:

CORAn	**corra(n,1), corra(n,2), ... corra(n,N)**
CORBn	**corrb(n,1), corrb(n,2), ... corrb(n,N)**
CORCn	**corrc(n,1), corrc(n,2), ... corrc(n,N)**

where the **CORAn**, **CORBn**, and **CORCn**, cards are used to describe the three coordinates as defined by the mesh type (rectangular, cylindrical or spherical), prior to any **trans** transformation.

In the case of rectangular meshes, **CORAn** represent planes perpendicular to the x-axis, **CORBn** are planes perpendicular to the y-axis, and **CORCn** are planes perpendicular to the z-axis. Bins do not have to be equally spaced.

In the case of the cylindrical mesh, the middle coordinate, **CORBn**, is the untransformed z-axis, which is the symmetry axis of the cylinder, with radial meshes defined in the **CORAn** input line. The first smallest radius may be equal to zero. The values following **CORBn** define planes perpendicular to the untransformed z-axis. The values following **CORCn** are positive angles relative to a counter-clockwise rotation about the untransformed z-axis. These angles, in degrees, are measured from the positive x-axis and must have at least one entry of 360, which is also required to be the last entry. The lower limit of zero degrees is implicit and never appears on the **CORCn** card.

In the case of spherical meshes, scoring will happen within a spherical volume, and can also be further defined to fall within a conical section defined by a polar angle (relative to the +z axis) and azimuthal angle. **CORAn** is the radius of the sphere, **CORBn** is the polar angle and **CORCn** is the same as in the cylindrical case. It is helpful in setting up spherical problems to think of the longitude-latitude coordinates on a globe.

The original capability of MCNP involving the “i” option is retained, allowing a large number of regularly spaced mesh points to be defined with a minimum of entries on the coordinate lines. All of the coordinate entries must be monotonically increasing for the tally mesh features to work properly, but do not need to be equally spaced. It should be noted that the size of these meshes scales with the product of the number of entries for the three coordinates. Machine memory could become a problem for very large meshes with fine spacing.

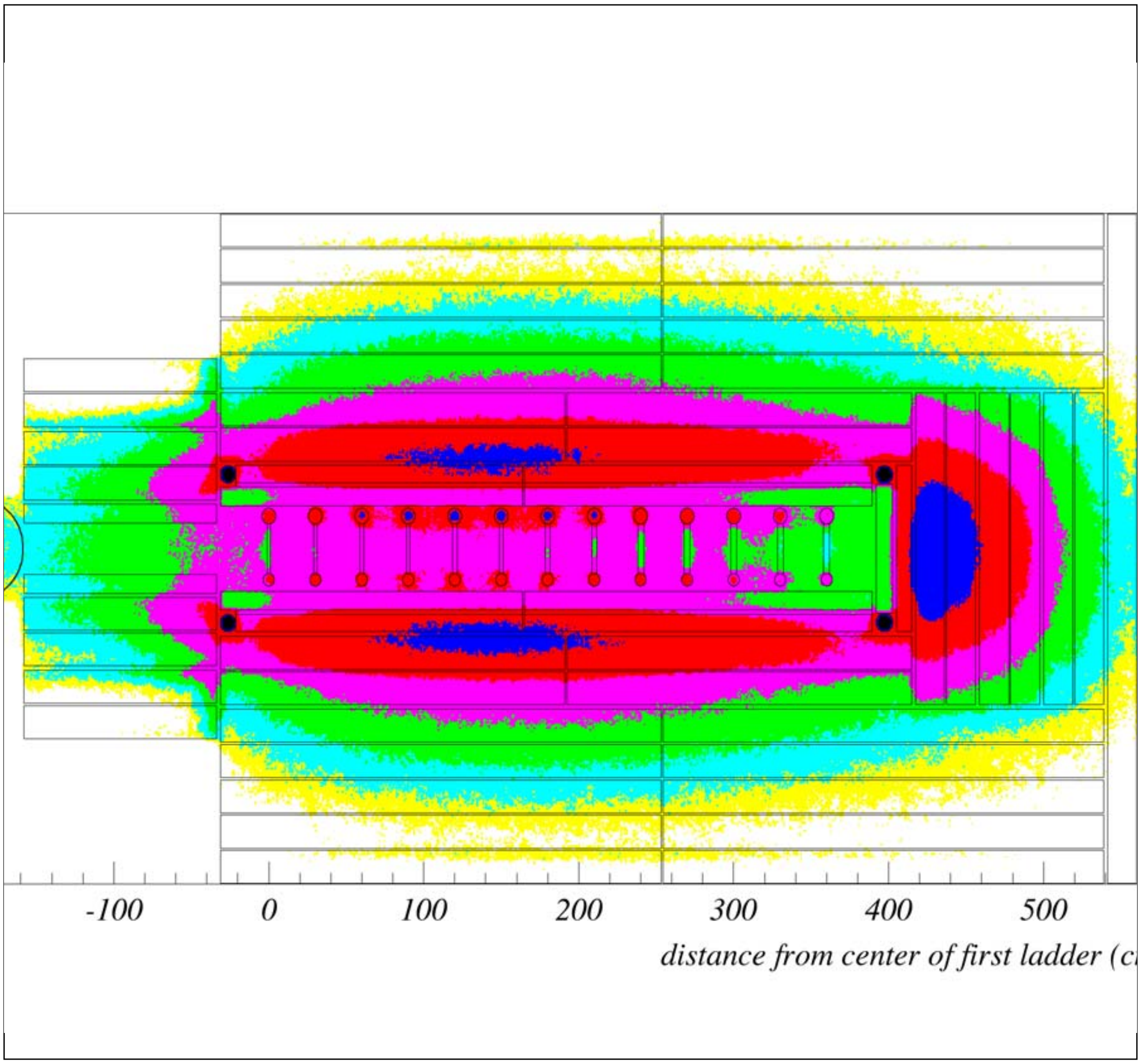


Figure 8-1. Mesh Tally depiction of a sample spallation target neutron fluence.

Additional cards which can be used with Mesh Tallies are:

ERGSHn E1 E2

MSHMFn **E1 F1 E2 F2 ...**
FMn **...**

Where **E1** is the lower energy limit for information to be stored to the mesh **n** and **E2** is the upper energy limit as they appear on the **ERGSH** card. The default is to consider all energies.

The entries on the **MSHMF** card are pairs of energies and the corresponding response functions; as many pairs can be designated as needed.

The **FM** card is the same as described in the MCNP4B users manual. Since it must be read and stored by the MCNP subroutines, it must not appear within the mesh data block between the **tmesh** and **endmd** cards.

The structure of the mesh as well as what quantities that are to be written to it are defined on two control cards in the MCNPX INP file. The general forms of the two mesh cards are:

RMESHn:P **keyword(i), i=1,10**
CMESHn:P **keyword(i), i=1,10**
SMESHn:P **keyword(i), i=1,10**

RMESH is a rectangular mesh, **CMESH** is a cylindrical mesh, and **SMESH** is a spherical mesh. The **n** is a user-defined mesh number. The last digit of **n** defines the type of information to be stored in the mesh[1]. **P** is the particle type being tallied, which be absent depending on the type of mesh tally. Up to 10 keywords are permitted, depending on mesh type. In MCNPX version 2.3.0, there are four general types of mesh tally cards, each with a different set of keywords.

[1] The user should be warned that the mesh tally number must be different from any other tally in the problem. For example, an f1:n tally will conflict with a RMESH1:n tally.

Track Averaged Mesh Tally (type 1)

The first mesh type scores track averaged data; flux, fluence or current. The values can be weighted by an **MSHMF** card, through the **DFACT** dose conversion coefficient function, or for energy deposition.

(R/C/S)MESHn:P **traks flux dose popul pedep mfact trans**

n = 1, 11, 21, 31,... (note, number must not duplicate one used for an 'F1' tally)

P is a particle type. There is no default. (see Table 5-1).

Table 8-1. Track-Averaged Mesh Tally (type 1) Keyword Descriptions

Keyword	Description
traks	The number of tracks through each mesh volume
flux	The average fluence is particle weight times track length divided by volume in units of number/cm^2. If the source is considered to be steady state in particles per second, then the value becomes flux in number/cm^2/second. (default)
dose	Causes the average flux to be modified by an energy dependent dose function. The "dose" keyword may be followed by up to four entries, where: • If the first entry is 1 to 9, an energy dependent dose function must be supplied by the user on a **MSHMF** card. • If the first entry is 10, 20, 31-35 or 40, the dose function comes from the function "dfact" (see Section 8.4 for details). The next three entries define the input needed by that function (the four needed entries correspond to **DFACT** arguments **ic**, **it**, **iu** and **acr**). • If no entries follow the dose keyword, the default entries are 10, 1, 1, and 1.0, which form inputs into the "dfact" function. Results are in rem/hour.
popul	Causes the population to be scored in each volume, which is equivalent to the weight times the track length.
pedep	Scores the average energy deposition per unit volume (MeV/cm^3/source-particle) for the particle type **P**. In contrast to the 3rd type of Mesh Tally, energy deposition can be obtained in this option for any particular particle. This option allows one to score the equivalent of an **F6:P** (see Section 8.3) heating tally for the particle type **P**. Note, the mesh is independent of problem geometry, and a mesh cell may cover regions of several different masses. Therefore the normalization of the **pedep** option is per mesh cell volume, not per unit mass.

Table 8-1. Track-Averaged Mesh Tally (type 1) Keyword Descriptions (Continued)

Keyword	Description
mfact	Can have from one to four numerical entries following it. • The value of the first entry is in reference to an energy dependent response function given on a MSHMFn card (no default). • The second entry is 1 (default =1) for linear interpolation, and 2 for logarithmic interpolation. • If the third entry is zero (default=0), the response is a function of energy deposited, otherwise the response is a function of the current particle energy. • The fourth entry is a constant multiplier and is the only floating point entry allowed (default=1.0). If any of the last three entries are used, the entries preceding it must be present so that the order of the entries is preserved. Only one **mfact** keyword may be used per tally.
trans	Must be followed by a single reference to a TR card that can be used to translate and/or rotate the entire mesh. Only one TR card is permitted with a mesh card.

Source Mesh Tally (type 2)

The second type of Mesh Tally scores source point data, in which the weight of the source particles **P(1), P(2), P(3), ...** are scored in mesh arrays 1, 2, 3, ..., therefore a separate mesh tally grid will be produced for each particle chosen. Currently it is not possible to chose more than one particle type in a type 2 Mesh Tally[1]. However some graphics programs will enable the user to add separate histograms together offline.

The usefulness of this method involves locating the source of particles entering a certain volume, or crossing a certain surface. The user asks the question, "If particles of a certain type are present, where did they originally come from?" In shielding problems, the user can then try to shield the particles at their source. Refinements in this tally will be forthcoming in further versions of MCNPX as user feedback is received.

This mesh tally is normalized as number per **SDEF** source particle.

(R/C/S)MESHn **P(1) P(2) P(3) P(4) ... trans**

n = 2, 12, 22, 32, ... (note, number must not duplicate one used for an 'F2' tally)

Table 8-2. Source Mesh Tally (type 2) Keyword Descriptions

Keyword	Description
P(i)	Particle type, i.e., n, p, e, etc., up to 10 particle types (see Table 5-1). Source particles are considered to be those that come directly from the source defined by the user, and those new particles created during nuclear interactions. One should be aware that storage requirements can get very large, very fast depending on the dimensions of the mesh, since a separate histogram is created for each particle chosen. If there are no entries on this card, the information for neutrons is scored by default.
trans	Must be followed by a single reference to a TR card that can be used to translate and/or rotate the entire mesh. Only one TR card is permitted with a mesh card.

[1] In MCNPX version 2.1.5, there was no option to chose individual particles. The type 2 Mesh Tally produced source points for all particles in the problem in one plot.

Energy Deposition Mesh Tally (type 3)

The third type of Mesh Tally scores energy deposition data in which the energy deposited per unit volume from all particles is included. This can be due to the slowing of a charged particle, the recoil of a nuclei, energy deposited locally for particles born but not tracked, etc. The results are similar to the scoring of an **+F6:np** tally as described in Section 8.3.

Note that in MCNPX version 2.3.0 the option to track energy deposition from one type of particle alone in a problem is included in the first Mesh Tally type (see Table 8-1, keyword **pedep**). The Energy Deposition Mesh Tally described here will give results for all particles tracked in the problem, and has no option to specify a particular particle. The request to track energy deposition by specific particle was received after this tally was developed, and therefore was included in the more convenient Mesh Tally type 1 **pedep** keyword.

Note, since the mesh is independent of problem geometry, a mesh cell may cover regions of several different masses. Therefore the normalization of the output is per mesh cell volume (MeV/cm^3/source-particle), not per unit mass.

(R/C/S)MESHn　　total de/dx recol tlest delct mfact nterg trans

n = 3, 13, 23, 33, ...

Table 8-3. Energy Deposition Mesh Tally (type 3) Keyword Descriptions

Keyword	Description
total, de/dx, recol, tlest, delct	Type of energy deposition scored: • total = energy deposited from any source (default) • de/dx = ionization from charged particles • recol = energy transferred to recoil nuclei above tabular limits • tlest = track length folded with tabular heating numbers • delct = non-tracked particles assumed to deposit energy locally

Table 8-3. Energy Deposition Mesh Tally (type 3) Keyword Descriptions (Continued)

Keyword	Description
mfact	Can have from one to four numerical entries following it. • The value of the first entry is in reference to an energy dependent response function given on a MSHMFn card (no default). • The second entry is 1 (default =1) for linear interpolation, and 2 for logarithmic interpolation. • If the third entry is zero (default=0), the response is a function of energy deposited, otherwise the response is a function of the current particle energy. • The fourth entry is a constant multiplier and is the only floating point entry allowed (default=1.0). If any of the last three entries are used, the entries preceding it must be present so that the order of the entries is preserved. Only one **mfact** keyword may be used per tally.
nterg	Allows one to record, in a separate mesh array, the local energy deposition only, due to particles otherwise not considered or tracked in this problem. This allows the user to ascertain the potential error in the problem caused by allowing energy from non-tracked particles to be deposited locally. This can be a serious problem in neglecting the tracking of high-energy photons or electrons.
trans	Must be followed by a single reference to a TR card that can be used to translate and/or rotate the entire mesh. Only one TR card is permitted with a mesh card.

DXTRAN Mesh Tally (type 4)

The fourth type of mesh tally scores the tracks contributing to all detectors defined in the input file for the **P** particle type. If this mesh card is preceded by an asterisk, tracks contributing to **DXTRAN** spheres are recorded. Obviously, a point detector or **DXTRAN** sphere must already be defined in the problem, and the tally will record tracks corresponding to all such defined items in the problem. The user should limit the geometrical boundaries of the grid to focus on a specific detector or **DXTRAN** sphere in order to prevent confusion with multiple detectors (although the convergence of the particle tracks should help in the interpretation).

This tally is an analytical tool useful in determining the behavior of detectors and how they may be effectively placed in the problem.

(R/C/S)MESHn:P **trans**

n = 4,14, 24, 34, ... (note, number must not duplicate one used for an ‘F4’ tally)

P is a particle type (neutron or photon). There is no default. (see table 5-1)

Table 8-4. DXTRAN Mesh Tally (type 4) Keyword Descriptions

Keyword	Description
trans	Must be followed by a single reference to a TR card that can be used to translate and/or rotate the entire mesh. Only one TR card is permitted with a mesh card.

8.1.2 Processing the Mesh Tally Results

The values of the coordinates, the tally quantity within each mesh bin, and the relative errors are all written by MCNPX to an unformatted binary file named **mdata**. This file is overwritten each time a dump is written to the **runtpe** file. Because of this overwrite, in doing a restart of MCNPX with a mesh tally, one must always use the last complete dump on the **runtpe** file.

The **gridconv** program is a post-processing code used with the **mdata** output file. It can also be used with the **mctal** output file from the radiography tally as described in Section 8.2. **Gridconv** converts the data arrays in **mdata** to forms compatible with various external graphics packages. Those supported in MCNPX version 2.3.0 are:

- **PAW** PAW (Physics Analysis Workstation) is distributed through the CERN Program Library. (http://wwwinfo.cern.ch/asd/paw/index.html)

- **IDL** IDL (Interactive Data Language) is a product of Research Systems, Inc., 4990 Pearl East Circle, Boulder, Co 80301 (http://www.rsinc.com/idl/index.cfm)
- **Tecplot** Tecplot is a product of Amtec Engineering, Inc., 13920 SE Eastgate Way, Ste. 220, Bellevue, Wa 98005 (http://www.amtec.com/)
- **GNUPLOT** Freeware - (http://www.gnuplot.info/). Only 1- and 2-d plots supported.

Like MCNPX, **gridconv** will compile on several platforms. However, currently the **PAW** part of the code will not compile on the Linux operating system, since some of the PAW subroutines needed by the code are not Linux compatible. **Gridconv** may be compiled with a 'nopaw' option (see table 3.1)

Once **gridconv** is compiled, one need type only the word "gridconv" to execute the code. The code will then prompt the user for information that is required such as file type, file names, etc. In most cases the default value is used and a return is all that is necessary.

Once the header information from **mdata** has been read from the file, **gridconv** can either produce an ASCII file from a binary or generate the required graphics input files as requested by the user. (Note that the ASCII file contains raw data not normalized to the number of source particles.) The reason for the option to write an ASCII file is that sometimes, users will want to look at the numbers in the **mdata** file before doing any plotting, or check the numerical results for a test case. The ASCII option is also very useful for porting the **mdata** file to another computer platform, and for reading the data into graphics packages not currently supported by **gridconv**.

Gridconv is currently set up to generate one-, two-, or three-dimensional graphics input files with any combination of binning choices. Once the input file has been generated, **gridconv** gives the user the options of producing another file from the currently selected mesh tally, selecting a different mesh tally available on this mdata file or reading information from a different file. Of course there is always the option to exit the program.

The capabilities of **gridconv** have recently been expanded so that any and all tallies written to **mctal** can be processed. The code is still interactive, but now shows all tallies in the problem, from which any may be selected. The user has the option of generating one- or two-dimensional output. The user is then told about the bin structure so the one or two free variables may be selected. The energy is the default independent variable in the one-dimensional case. There is no default for the two-dimensional case. The order in which the two-dimensional bin variables are selected does not make any difference to the output, in that the order of the processing will be as it appears on the **mctal** file. **Gridconv** will work with mctal files produced both by MCNPX and MCNP.

8.2 The Radiography Tally

A capability has been added to MCNPX to allow the code to generate simulated radiography images as one would expect to see from an X-ray or pinhole projection of an object containing the particle source.This allows the recording of both the direct (source) image as well as that due to background (scatter). This tool is an invaluable aid to the problem of image enhancement, or extracting the source image from a background of clutter. MCNPX includes two types of image capability; the pinhole image projection and the transmitted image projection.

The radiography capability is based on point detector techniques, and is extensively described in SNO96 and SNO98. In essence, the radiography focal plane grid is an array of point detectors.

8.2.1 Pinhole Image Projection

In the pinhole image projection case, a point is defined in space that acts much like the hole in a pinhole camera and is used to focus an image onto a grid which acts much like the photographic film. The pinhole is actually a point detector and is used to define the direction cosines of the contribution that is to be made to the grid. The pinhole position relative to the grid is also used to define the element of the grid into which this contribution is scored. Once the direction is established, a ray-trace contribution is made to the grid bin with attenuation being determined for the material regions along that path. The source need not be within the object being imaged, nor does it need to produce the same type of particles that the detector grid has been programmed to score. The grid and pinhole will image either source or scattered events produced within the object (see **NOTRN** card in Section 8.2.3) for either photons or neutrons. These event type contributions can be binned within the grid tallies by binning as source only, total, or by using special binning relative to the number of collisions contributing cells, etc.

The pinhole image projection is set up as follows in version 2.1.5:

FIn:P X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3

In MCNPX version 2.3.0, the form of the card has been changed (old input files are backward compatible if one replaces the control card symbol):

PIn:P X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3

n is the tally number and must be a multiple of 5 since this is a detector-type tally.

P is the particle type for the tally. Only neutrons or photons are allowed, since detector techniques do not currently work for charged particles.

Table 8-5. Pinhole Radiography Argument Descriptions

Argument	Description
X1, Y1, Z1	The coordinates of the pinhole.
R0	Always 0 (zero) for this application. Note, neither the pinhole nor the grid should be located within a highly scattering media.
X2, Y2, Z2	The reference coordinates that establish the reference direction cosines for the normal to the detector grid. This direction is defined as being from **X2, Y2, Z2** to the pinhole at **X1, Y1, Z1**.
F1	If **F1**>0, the radius of a cylindrical collimator, centered on and parallel to the reference direction, which establishes a radial field of view through the object.
F2	The radius of the pinhole perpendicular to the reference direction. • **F2**=0 represents a perfect pinhole • **F2**>0 the point through which the particle contribution will pass is picked randomly. This simulates a less-than-perfect pinhole.
F3	The distance from the pinhole at **X1, Y1, Z1** to the detector grid along the direction established from **X2, Y2, Z2** to **X1, Y1, Z1**, and perpendicular to this reference vector.

The grid dimensions are established from entries on **FS** and **C** cards.In this use, the first entry sets the lower limit of the first bin, and the other entries set the upper limit of each of the bins. These limits are set relative to the intersection of the reference direction and the grid plane as shown in Figure 8-2.

An example is discussed below:

FSn -20. 99i 20.

Cn -20. 99i 20.

These two cards set up a 100 x 100 grid that extends from -20 cm to 20 cm in both directions, and has 10,000 equal size bins. These bins need not be equal in size nor do they need to be symmetric about the reference direction.

The directions of the t-axis and s-axis of the grid are set up such that if the reference direction (the outward normal to the grid plane), is not parallel to the z-axis of the geometry, the t-axis of the grid is defined by the intersection of the grid plane and plane formed by the z-axis and the point where the reference direction would intersect the grid plane. If the reference direction is parallel to the z-axis of the geometry, then the t-axis of the grid is defined to be parallel to the y-axis of the geometry. The x-axis of the grid is defined as the cross product of a unit vector in the “t" direction and a unit vector in the reference direction.

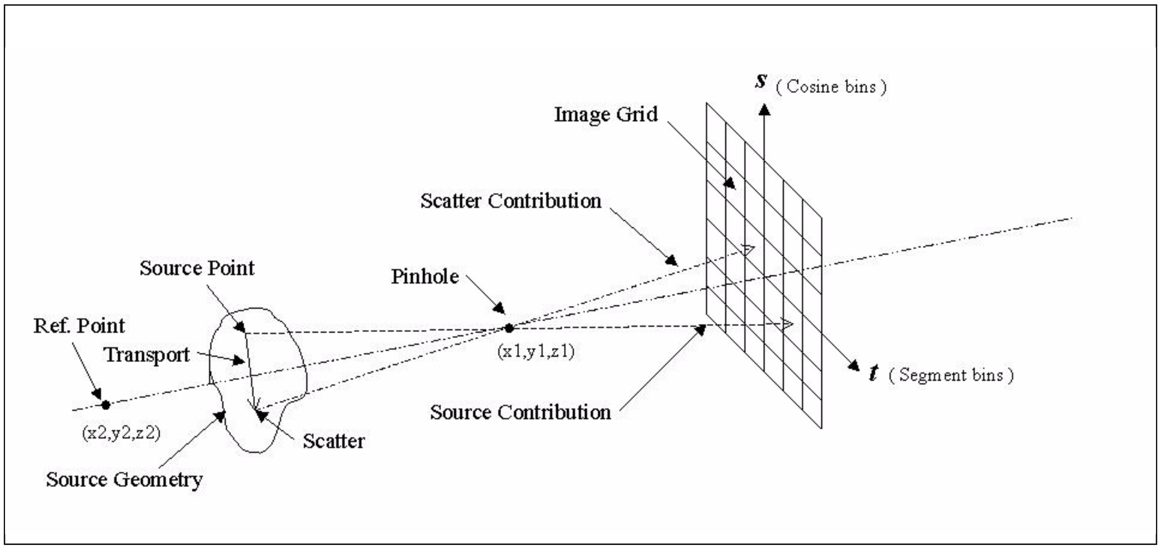


Figure 8-2. Pinhole image projection.

8.2.2 Transmitted Image Projection

In the transmitted image projection case, the grid acts like a film pack in an X-ray type image, or transmitted image projection. The diagram in figure 8.3 shows how the planar grid type of image capability is set up. In MCNPX 2.3.0 additional capability has been added to allow the user to set up a cylindrical grid for generating an image. In both cases, for every source or scatter event a ray-trace contribution is made to every bin in the detector grid. This eliminates statistical fluctuations across the grid that would occur if the grid location of the contribution from each event were to be picked randomly, as would be the case if one used a **DXTRAN** sphere and a segmented surface tally. For each event, source or scatter, the direction to each of the grid points is determined, and an attenuated ray-trace contribution is made. As in pinhole image projection, there are no restrictions as to location or type of source used. These tallies automatically bin in a source-only and a total contribution, but could be further binned as described for the pinhole tally.

The transmitted image projection is set up as follows in version 2.1.5:

FIn:P X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3

Note that this form is the same as the pinhole image. The transmitted image capability is turned on by setting F2 less than zero, as described below.

Version 2.3.0 changes the form of the card (old input files are backward compatible if one replaces the control card symbol):

TI(R/C)n:P X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3

TIR is used to establish a grid on a plane surface

TIC is used to establish a grid on a cylindrical surface.

n is the tally number and must be a multiple of 5 since this is a detector-type tally.

P is the particle type for the tally. Only neutrons or photons are allowed, since detector techniques do not currently work for charged particles.

Table 8-6. Transmitted Image Projection Argument Description

Argument	Description
X1, Y1, Z1	The coordinates used with the entries on the **FSn** and **Cn** cards to define the detector grid. In the plane grid case, this defines the center of the grid. In the cylindrical grid case, this defines the center of the cylinder on which the grid is established.
R0	Always 0 (zero) in this application, as in the pinhole case.
X2, Y2, Z2	The reference coordinates that establish the reference direction cosines for the outward normal to the detector grid plane, as from **X2**, **Y2, Z2** to **X1, Y1, Z1**. This is used as the outward normal to the detector grid plane for the **TIR** case, and as the centerline of the cylinder for the **TIC** case.
F1	• **F1=0** Both the source and scattered contributions will be scored at the grid. • **F1<0** Only the scatter contributions will be scored. • **F1>0** is not allowed in this application.
F2	**F2** must be less than 0 to turn on this type of image application in 2.1.5. This restriction has been removed in 2.3.0. Do not make **F2**=0 as this will result in a fatal error. *plane grid case*: Radial restriction relative to the center of the grid for contributions to be made. It defines a radial field of view on the grid. *cylindrical case*: Radius of the cylinder on which the grid is to be established.
F3	**F3 = 0** All contributions are directed to the center of each grid bin. **F3 < 0** Contributions are made with a random offset from the center of the grid bin. This offset remains fixed and is used as the offset for contributions toll of the grid bins for this event.

The grid itself is established with the use of **FSn** and **Cn** cards in the same manner as described for the pinhole case in Section 8.2.1. However, **X1**, **Y1**, **Z1** are now the coordinates of the intersection of the reference direction and the grid plane as shown in Fig. 8-3. In the cylindrical grid case, the entries on the **FSn** card are the distances along the symmetry axis of the cylinder and the entries on the **Cn** card are the angles in degrees as measured counterclockwise from the positive t-axis.

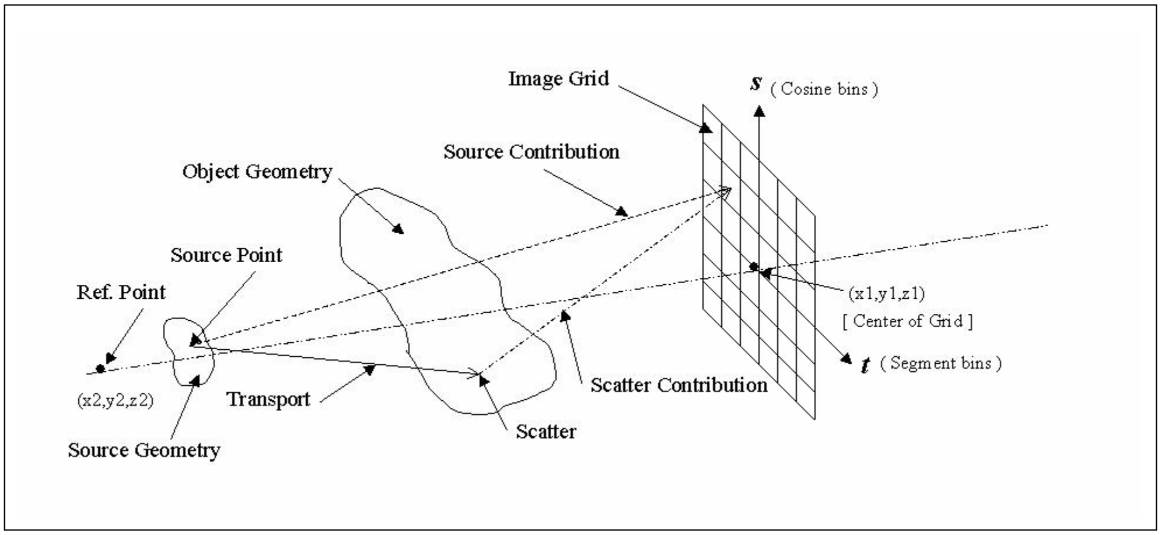


Figure 8-3. Transmitted image projection.

When this type of detector is being used in a problem, if a contribution is required from a source or scatter event, an attenuated contribution is made to each and every detector grid bin. Since for some types of source distributions, very few histories are required to image the direct or source contributions, an additional entry has been added to the NPS card to eliminate unwanted duplication of information from the source. The new NPS card now becomes:

NPS NPP NPSMG

Table 8-7. NPS Keyword Descriptions

Keyword	Description
NPP	Total number of histories to be run in the problem.
NPSMG	Number of histories for which source contributions are to be made to the detector grid.

When the number of source histories exceeds **NPSMG**, the time consuming process of determining the attenuation of the direct contribution is avoided by adding the average of the previous direct contributions into each of the appropriate tally bins. Depending on the time required for a particular problem, this can save from a few seconds to upward of ten minutes per history in some cases. As described above, for a monoenergetic isotropic point source, or a monoenergetic monodirectional surface source, **NPSMG**=1 is adequate.

8.2.3 Additional Radiography Input Cards

A **NOTRN** card is added as an additional possible input. When this card appears in the **INP** file, no transport of the source particles takes place, and only the direct or source contributions are made to the detector grid. This is especially useful for checking the problem setup or doing a fast calculation to generate the direct source image. This option works with either the pinhole or transmitted image options.

The option is also available to turn off the printing of all of the values in each of the grid bins in the **OUTP** file. The card **TALNP** with no arguments turns off the bin print for all tallies in the problem. If there are entries, it turns off the bin print for the tally numbers that are listed. If, after the run is completed, one would like to see these numbers, the printing of the bin values can be restored with the **TALNP** card in an **INP** file used in a continue run. The tally numbers are entered on the **TALNP** card as negative numbers.

8.2.4 Reading the Radiography Tally Output

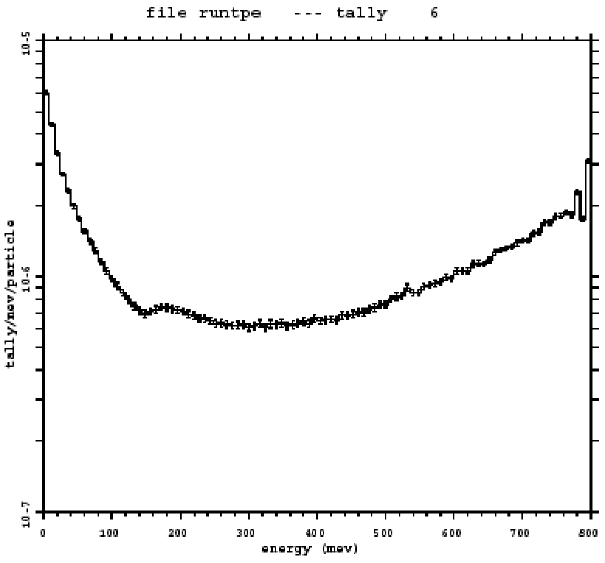
The output of the two radiography tally options is contained in the **mctal** file. It can be formatted for use with external graphics programs with the **gridconv** routine. The user is referred to Section 8.1.2 for information on how to use **gridconv**.

8.3 Energy Deposition

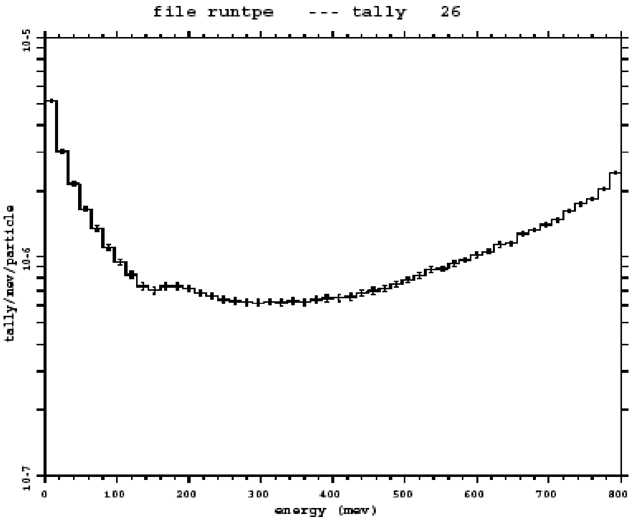
With the high energy extensions in MCNPX, considerable thought has gone into the design and adoption of energy deposition tallies. In particular, we must address such issues as:

- Local energy deposition of non-tracked particles is not valid as particle energy increases.
- Heating numbers and Kerma factors do not exist in the physics modules. Energy deposition processes must be modeled online as interactions occur, and the individual contributions summed. This process is termed 'collision based' estimate.
- Track ionization for charged particles is not linearly distributed over a step, but can increase or decrease as the particle slows down, depending on initial energy. MCNPX 2.3.0 always scores the energy of a particle at the beginning of a step. In most cases, step sizes for charged particles are small, therefore little error is introduced in this process.
- However, occasionally particles may lose so much energy in one transport step that they will skip over some energy bins set up in a tally, causing a 'picket fence' structure in energy spectra. Figure 8.4 illustrates this effect, which will show up in any spectra plotted as a function of energy for an 800 MeV proton beam hitting a tungsten target.

Figure 8.4 Effect of too fine binning on energy spectra
a) Proton Energy deposition spectra with 100 bins. Note the 'picket fence' effect at high energies.



b) Proton energy deposition spectra with 50 bins. 'Picket Fence' effect has disappeared.



The exact treatment of energy deposition depends on particle type.

Photons:

In a photon-only problem, the photon heating numbers are used to estimate the energy deposition as a function of track length in the cell. In cells where the electrons that would be produced cannot travel very far, this is a reasonably good approximation, since the use of heating numbers assumes that the energy from these "would-be" secondary particles is deposited locally. However, if the cells are "thin" to electron transport, this becomes a poor approximation, and one should use a coupled photon/electron mode to get better results. In fact, in working with these type of coupled problems, it was found that the most consistent results, as compared to a **F8:p,e** tally, could be achieved if the energy deposited by the electrons only was scored. This seems to work very well since in photon energy deposition, most if not all of the energy lost by the photon goes into creating secondary electrons that then account for the energy deposited in the cell.

Electrons:

The electron energy deposition is evaluated as the de/dx ionization, uniformly distributed along track length dx. Then several adjustments are made, the first of which is for x-ray production if photons are to be produced (by including a **p** on the **mode** card). The de/dx term is decreased by the amount of energy that goes into the secondary x-rays produced if they are being transported, otherwise this adjustment is not made. An adjustment is always made for the knock-on electrons or delta rays produced, since these will be banked and subsequently transported and their energy deposited during that transport process. There are also adjustments made for any auger electrons produced. In addition, if the bremsstrahlung photons are not to be transported, the electron energy that would be lost in their production is also distributed uniformly along the electron particle track. Of course, if these photons are to be transported, no corrections to the electron energy deposition is made.

Heavy Neutral and Charged Particles:

In the energy range where tables are available, the neutron and proton energy deposition is determined using the neutron heating numbers in the same manner as **F6** tallies are done in MCNP4B. These heating numbers are estimates of the energy deposited per unit track length. In addition, the de/dx ionization contribution for the proton is added in, similar to the electron treatment.

Above that tabular energy limit, or when no tabular data is available, energy deposition is determined by summing several factors. For charged particles, ionization (de/dx) energy is deposited uniformly along the track length (which is important to keep in mind when doing a mesh tally). All other energy deposition is calculated at the time of a nuclear interaction. The energies of secondary particles, if they are not to be tracked (i.e., not included on the **MODE** card) will be deposited at the point of the interaction. Nuclear recoil energy will always be deposited at the point of interaction.[1]

In order to obtain the most accurate energy deposition tallies possible, the user must include all potential secondary particles on the **MODE** card. (Electrons can be omitted, provided the user fully understands how energy deposition for photons is done.) The handling of energy deposition for non-tracked secondary particles differs for the energies where libraries and physics models are used. This procedure is under review and will likely be changed in future versions of the code.

Energies of all secondary particles except photons are added into the heating/KERMA factors for the neutron and proton libraries. This photon treatment was implemented in the MCNP libraries well before the development of the MCNPX code. However, since MCNP4B does not track charged particles, standard practice was to include the energies of all other particles in the heating numbers for the evaluated libraries. We are increasingly finding that local deposition of secondary particle energies causes difficulties, particularly when the energies of the secondaries are high, or when the user is simulating thin volumes. When secondary particles are indicated on the MODE card, MCNPX will subtract

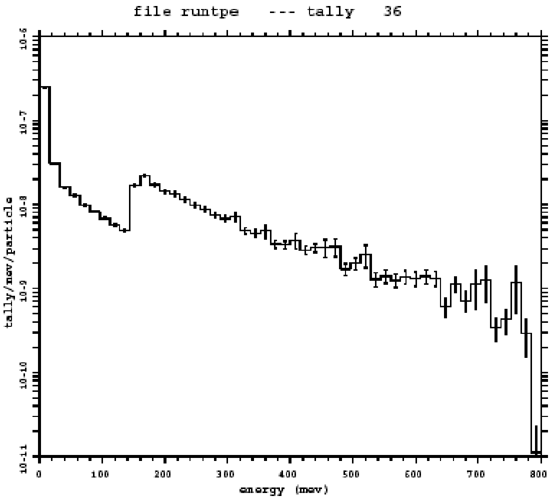
[1] In MCNPX version 2.3.0, residual nuclei cannot be tracked. This is usually not a problem for heavy residuals, however for light residuals, (such as a scattered hydrogen nucleus), errors in energy deposition in small volumes can occur. This has caused some users problems when tracking in small volumes where it is unlikely that the recoil hydrogen nucleus will not stop. We will modify this practice in an upcoming release.

their energies from the heating values, and energy deposition will be handled in the regular process of tracking those particles[1].

Where there are no libraries available, de/dx, nuclear recoil, and the energies of some non-tracked secondary particles are added to the F6 collision estimator. A secondary particle can be produced either by collision or by particle decay[2]. In MCNPX version 2.3.0, the energies of neutral particles will never be added to the collision estimator (this includes neutrons, photons, neutrinos, pi0 and neutral Kaons). This is not consistent with the library heating factor treatment, and will be reconsidered in future versions of the code. Therefore, it is especially important for the user to include all possible secondary particles on the MODE card (especially photons and neutrinos), in order to get the most accurate energy deposition tally. Figure 8.5 illustrates the difference in an energy spectra for neutrons on a tungsten target when photons are not (8.5a), or are (8.5b) included in the **MODE** card. The difference made by tracking the photons is substantial.

Figure 8.4 **Energy Deposition Spectra for Neutrons produced by an 800 MeV proton beam on Tungsten**

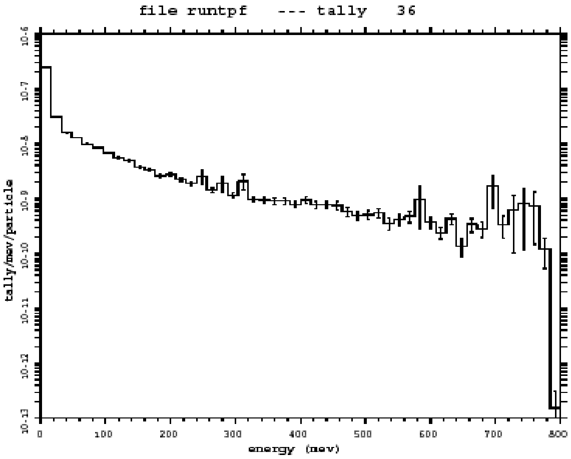
a) MODE h n / | d t s a u



[1] Energies of particles which fall below minimum energy cutoffs will also be deposited locally. The user must be certain that the value of these cutoff energies will not cause the results of the F6 tally to be in error.

[2] Note that the Pi^0, if included on the MODE card, will be transported before it decays, even though its lifetime is 8.4×10^{-17} seconds. This allows the user to use MCNPX tallies for that particle.

b) mode h n p / | d t s a u



In MCNPX version 2.3.0, the two forms of the **F6** tally are:

F6:P **C1 C2 ... Cm**
+F6 **C1 C2 ... Cm**

Table 8-8. Energy Deposition Card Argument Descriptions

Argument	Description
C1, C2, ...	Cell numbers in which to score energy deposition.

MCNPX has the standard **F6n:P** tally, where **P** can now be any particle. In addition, MCNPX has a new **+F6n** tally, which contains energy deposition from all particles in the problem. It is not currently possible to have an **F6** tally which will do energy deposition for more than one, but less than all particles. We will consider adding this capability in the future. Note that the pedep keyword in a Type 1 Mesh Tally is analogous to the **F6n:P** tally, and the Type 3 Mesh Tally is analogous to the **+F6n** tally, although the normalizations will be different. Since the mesh tallies score energy deposition within a mesh cell, which may contain more than one material, normalization is The units of this tally are MeV/source-particle. In the **F6** and **+F6** tallies, material density is available for the chosen cells, and normalization is MeV/gm/source-particle.

8.4 Dose Conversion Coefficients

The health physics industry and regulatory authorities have published a variety of fluence-to-dose conversion coefficients, and it can be difficult for the unexperienced user to keep track of the latest versions. In addition, much new work is in progress for providing coefficients for particles other neutrons and photons, as well as extending the limits of their upper ranges to the high energies needed in many accelerator applications.

A new function has been added to MCNPX, which contains a number of standard dose conversion coefficients, and efforts are being made to include the option to call this function in various tallies. In MCNPX version 2.3.0, this function is directly used through the **dose** keyword of the Type 1 Mesh Tally (section 8.1.1).

If access to the MCNPX source code is available, the user can add additional factors, although this can also be done by individually inputting values into the de/dfcards. Function **DFACT** is an effort to hardwire in standard values, since user input can be notoriously subject to error. The MCNPX code developers will add more options as they become available. The **acr** option can also be modified to add user-defined response functions for dosimetry monitoring devices.

function DFACT(id, ic, en, it, iu, acr)

Table 8-9. DFACT Argument Descriptions

ARGUMENT	DESCRIPTION
id	Particle identification number: 1 = neutron 2 = photon
ic	Choice of conversion coefficient. Note: The 10 and 20 options are Dose Equivalent (H), i.e., absorbed dose at a point in tissue weighted by a distribution of quality factors (Q) related to the LET distribution of radiation at that point. The 30’s options are Equivalent Dose ($H_{t)}$ based on an average absorbed dose in the tissue or organ ($D_{t)}$, weighted by the radiation weighting factor (w_r), summed over all component radiations. neutrons: 10 = ICRP-21 1971 20 = NCRP-38 1971, ANSI/ANS 6.1.1 - 1977 31 = ANSI/ANS 6.1.1 - 1991 (AP anterior-posterior) 32 = ANSI/ANS 6.1.1 - 1991 (PA posterior-anterior) 33 = ANSI/ANS 6.1.1 - 1991 (LAT side exposure) 34 = ANSI/ANS 6.1.1 - 1991 (ROT normal to length & rotationally symmetric) 40 = ICRP-74 1996 ambient dose equivalent photons 10 = ICRP-21 1971 20 = Claiborne & Trubey, ANSI/ANS 6.1.1-1997 31 = ANSI/ANS 6.1.1 - 1991 (AP anterior-posterior) 32 = ANSI/ANS 6.1.1 - 1991 (PA posterior-anterior) 33 = ANSI/ANS 6.1.1 - 1991 (LAT side exposure) 34 = ANSI/ANS 6.1.1 - 1991 (ROT normal to length & rotationally symmetric) 35 = ANSI/ANS 6.1.1 - 1991 (ISO isotropic)
en	Particle energy
it	Interpolation method 1 = logarithmic interpolation in energy, linear in function 2 = linear interpolation in energy and function 3 = recommended analytic parameterization (not available for ic=10)
iu	units of the result 1 = (rem/hr)/(particles/cm^2-sec) 2 = (sieverts/hr)/(particles/cm^2-sec)

Table 8-9. DFACT Argument Descriptions (Continued)

ARGUMENT	DESCRIPTION
acr	Normalization factor for dose. DFACT result will be multiplied by any factor greater or equal to 0.0 (for example, acr=1.0 means no change). The value must be a real number. Certain special options are also available. -1.0 = normalize DFACT results to Q=20 by dividing out the parametric form of Q, which equals 5.0+17.0*exp(-(ln(2E))/*2/6) from ICRP60 (1990), paragraph A12. -2.0 = Apply LANSCE albatross response function.

8.5 HISTP and HTAPE3X

In order to produce the LAHET - compatible HISTP files, the following card must be added to the inp deck:

HISTP (no arguments)

HTAPE3X is a code for processing medium-and high-energy collision data written to the HISTP history file by MCNPX. In addition it provides surface flux and current edits which supplement the standard MCNP tallies. HTAPE3X is an adaptation of the LAHET Code System HTAPE code. Details may be found in User Guide to LCS (PRA89), and the manual as written for use in MCNPX is reproduced in Appendix B of this document.

The user should note the following comments, since HTAPE3X does not contain any provision for many of the termination options allowed by MCNPX which affect the content of the HISTP file. The user must be aware of the possible implications on normalization of outputs. HTAPE3X will correctly process HISTP for the following cases:

1. Normal completion after **NPS** histories. **N=NPS** is used for the degrees of freedom in the statistical analysis to compute means and variances.
2. Termination is by **(^c)k** or “system crash;” HISTP lacks a final record. **N** is taken to be the highest observed history number; this is a good approximation if **N** is large and most histories contribute to the HISTP file.

However, other modes of termination of the MCNPX produce the following results:

3. Termination by **(^c)q** with NPS input record present: The correct **N** is unknown to HTAPE3X and **NPS** is used. The user may normalize the HTAPE3X output by the ratio **NPS/N**, but the calculated variances will not reflect this correction.
4. Termination on time using **CTME**, when **NPS** input record is present. See comment #3 above.
5. If an NPS record is absent, HTAPE3X will crash in the termination stage; HISTP may be edited as noted in comment #3 above.

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Appendix A – Examples

Example 1: Neutron production from a spallation target

One of the fundamental quantities of interest in most spallation target applications is the number of neutrons produced per beam particle incident on target. For targets fed by proton accelerators, this quantity is typically denoted as "n/p”. Here, we demonstrate how one goes about calculating this quantity for a simple target geometry using MCNPX.

The geometry consists of a simple right-circular cylinder of lead, 10 cm in diameter by 30 cm long. A beam of 1-GeV protons is launched onto the target. The beam has a spot size of 7-cm diameter, with a parabolic spatial profile (see Fig. A-1).

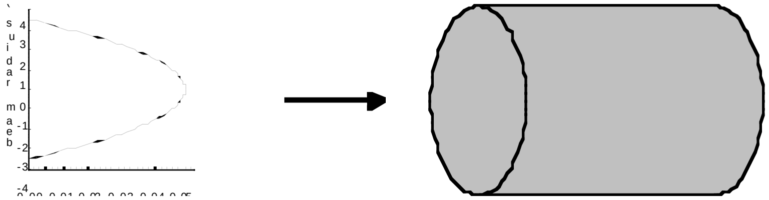

Figure A-1. Neutron production from a spallation target.

In MCNPX, net neutron production is tallied implicitly and is provided by default in the problem summary for neutrons. The problem summary shows net neutron production resulting from nuclear interactions (this is the component that accounts for neutron production by all particles transported using INC/Preequilibrium/Evaporation physics), and net production by (n,xn) reactions (these are neutrons created in inelastic nuclear interactions by neutrons below the transition energy, using evaluated nuclear data). Net production from nuclear interactions is given by the difference of the neutron weights in the "neutron creation" and "neutron loss" columns. A similar approach is taken to calculate net (n,xn) production. Net neutron production may also be calculated by realizing that the only loss mechanisms for neutrons are escape and capture. The sum of the weights in the "neutron loss" column under "escape" and "capture" is thus equal to the net neutron production. The values listed in the problem summary are "collision estimators," meaning they are tallied when a collision occurs during transport. Uncertainties are not calculated by MNCPX for these collision-estimated quantities. A reasonable upper limit on the relative uncertainty would be given by the inverse square root of the number of source particles launched.

We provide here five different variations for the calculation of net neutron production for this simple target geometry. In the "base case," we transport protons, neutrons, and charged pions. The transition energy between LAHET physics and neutron transport using tabular nuclear data is set at 150 MeV, and the LA150 library is used. All protons are transported using LAHET physics. Nucleon and pion interactions simulated by LAHET physics use the Bertini intranuclear cascade model. Variations from this base case are outlined in Table A-1 below. For each case, 20,000 source protons were transported.

Table A-1. Neutron Problem Summaries

Case	INC Model	Particles transported	Neutron transition energy (MeV)	Proton transition energy (MeV)
base	Bertini	n h /	150	0
1	Bertini	n h /	20	0
2	Bertini	n h / d t s a	150	0
3	ISABEL	n h /	150	0
4	Bertini	n h /	150	150
5	CEM	n h /	150	0

For the sake of brevity, we reproduce here just the neutron problem summaries from the MCNPX output decks.

Base Case

```
sample problem: spallation target
c    neutron production with 20-MeV neutron transition energy
c    EJ Pitcher, 1 Nov 99
c
c    --- cell cards ---
c
c    Pb target
   1 1 -11.4   1 -2 -3
c    bounding sphere
   2 0        (-1:2:3) -4
c    outside universe
   3 0         4

c    --- surface cards ---
c
   1   pz  0.0
   2   pz 30.0
   3   cz  5.0
```

```
    4   so 90.0

c      --- material cards ---
c
c      Material #1: Pb without Pb-204
m1     82206.24c 0.255 82207.24c 0.221 82208.24c 0.524
c
c      --- data cards ---
mode n h /
imp:n,h,/ 1 1r 0
phys:n 1000. j 150.
phys:h 1000. j 0.
lca j j j
nps    20000
prdmp  j -30 j 1
c
c     --- source definition ---
c     1-GeV proton beam, 7-cm-diam, parabolic spatial profile
sdef   sur 1 erg 1000. dir 1 vec 0. 0. 1. rad d1 pos 0. 0. 0. par 9
si1  a   0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3
         1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2 2.3 2.4 2.5 2.6 2.7
         2.8 2.9 3.0 3.1 3.2 3.3 3.4 3.5
sp1      0.00000 0.09992 0.19935 0.29780 0.39478 0.48980 0.58237
         0.67200 0.75820 0.84049 0.91837 0.99135 1.05894 1.12065
         1.17600 1.22449 1.26563 1.29894 1.32392 1.34008 1.34694
         1.34400 1.33078 1.30678 1.27151 1.22449 1.16522 1.09322
         1.00800 0.90906 0.79592 0.66808 0.52506 0.36637 0.19151
         0.00000
```

For the base case, the neutron problem summary follows:

```
      sample problem: spallation target base case
neutron creation       tracks   weight        energy           neutron loss           tracks   weight        energy
                                 (per source particle)                                          (per source particle)

 source                    0    0.            0.                   escape              365317    1.8249E+01    2.1995E+02
 nucl. interaction    316017    1.5801E+01    3.2136E+02           energy cutoff            0    0.            0.
 particle decay            0    0.            0.                   time cutoff              0    0.            0.
 weight window             0    0.            0.                   weight window            0    0.            0.
 cell importance           0    0.            0.                   cell importance          0    0.            0.
 weight cutoff             0    0.            0.                   weight cutoff            0    0.            0.
 energy importance         0    0.            0.                   energy importance        0    0.            0.
 dxtran                    0    0.            0.                   dxtran                   0    0.            0.
 forced collisions         0    0.            0.                   forced collisions        0    0.            0.
 exp. transform            0    0.            0.                   exp. transform           0    0.            0.
 upscattering              0    0.            0.                   downscattering           0    0.            9.8498E+00
 tabular sampling          0    0.            0.                   capture                  0    1.4266E-02    7.6455E-02
 (n,xn)                78320    3.9123E+00    1.8804E+01           loss to (n,xn)       25352    1.2660E+00    4.8878E+01
 fission                   0    0.            0.                   loss to fission          0    0.            0.
 photonuclear              0    0.            0.                   nucl. interaction     3668    1.8340E-01    6.1409E+01
 tabular boundary          0    0.            0.                   tabular boundary         0    0.            0.
 (gamma,xn)                0    0.            0.                   particle decay           0    0.            0.
 adjoint splitting         0    0.            0.
     total            394337    1.9713E+01    3.4016E+02               total           394337    1.9713E+01    3.4016E+02

  number of neutrons banked                   368985        average time of (shakes)              cutoffs
 neutron tracks per source particle      1.9717E+01          escape           5.7458E+00          tco   1.0000E+34
 neutron collisions per source particle  2.7874E+01          capture          4.6648E-01          eco   0.0000E+00
 total neutron collisions                    557485          capture or escape 5.7417E+00          wc1  -5.0000E-01
 net multiplication              0.0000E+00  .0000          any termination   5.3201E+00          wc2  -2.5000E-01
```

-The two methods for calculating total neutron production give the following results:

net nuclear interactions + net (n,xn):	(15.801 - 0.1834) + (3.9123 - 1.2660)	= 18.263 n/p
escapes + captures:	18.249 + 0.014226	= 18.263 n/p

Both methods give the same answer. Since "escapes + captures" is easier to calculate, this is the method typically used. A reasonable upper limit on the relative uncertainty of n/p is (20,000) ~ 0.7%.

Case 1

The first variation considered is the impact of the extension of the evaluated neutron cross sections to 150 MeV on total neutron production. To evaluate this impact, we set the transition energy between LAHET physics and neutron transport using evaluated nuclear data (given by the third value on the phys:n card) to 20 MeV:

Base Case: `phys:n   1000. j 150.`
Case 1: `phys:n    1000. j 20.`

In this case, neutron transport is done in the same manner as was done traditionally with LAHET and HMCNP. The neutron problem summary for this case is shown below.

```
      sample problem: spallation target: Case 1

neutron creation       tracks   weight        energy            neutron loss           tracks   weight        energy
                                 (per source particle)                                           (per source particle)

 source                     0    0.           0.                 escape              367324    1.8351E+01    2.1946E+02
 nucl. interaction     376685    1.8834E+01    3.3940E+02        energy cutoff            0    0.            0.
 particle decay             0    0.           0.                 time cutoff              0    0.            0.
 weight window              0    0.           0.                 weight window            0    0.            0.
 cell importance            0    0.           0.                 cell importance          0    0.            0.
 weight cutoff              0    0.           0.                 weight cutoff            0    0.            0.
 energy importance          0    0.           0.                 energy importance        0    0.            0.
 dxtran                     0    0.           0.                 dxtran                   0    0.            0.
 forced collisions          0    0.           0.                 forced collisions        0    0.            0.
 exp. transform             0    0.           0.                 exp. transform           0    0.            0.
 upscattering               0    0.           0.                 downscattering           0    0.            9.8003E+00
 tabular sampling           0    0.           0.                 capture                  0    1.3626E-02    5.7541E-02
 (n,xn)                 20323    1.0137E+00    1.5895E+00        loss to (n,xn)        9964    4.9705E-01    6.8449E+00
 fission                    0    0.           0.                 loss to fission          0    0.            0.
 photonuclear               0    0.           0.                 nucl. interaction    19720    9.8600E-01    1.0482E+02
 tabular boundary          11    5.5000E-04    1.0972E-02        tabular boundary        11    5.5000E-04    1.0972E-02
 (gamma,xn)                 0    0.           0.                 particle decay           0    0.            0.
 adjoint splitting          0    0.           0.
     total             397019    1.9848E+01    3.4100E+02            total           397019    1.9848E+01    3.4100E+02

  number of neutrons banked                   387055        average time of (shakes)              cutoffs
  neutron tracks per source particle      1.9851E+01          escape           5.8655E+00          tco   1.0000E+34
  neutron collisions per source particle  2.8027E+01          capture          4.8948E-01          eco   0.0000E+00
  total neutron collisions                    560536          capture or escape 5.8615E+00          wc1  -5.0000E-01
  net multiplication              0.0000E+00  .0000          any termination   5.4273E+00          wc2  -2.5000E-01
```

Net neutron production in this case is 18.364 n/p, or 0.5% above the base case value. The difference is primarily due to the neutron multiplicity between 20 and 150 MeV in the new 150-MeV evaluations as compared to the multiplicity given by the LAHET physics models in this energy range. Since the data evaluations are considered more accurate than the LAHET physics models, the base case value of 18.263 should be considered the better estimate.

Note the difference in net production by nuclear interactions (15.617 n/p for the base case versus 17.897 n/p for case 1) and by (n,xn) reactions (3.785 n/p for the base case versus 0.516 n/p for case 1) for the two cases. The difference of 2.280 n/p between the two cases for net production by nuclear interactions is the value calculated by the LAHET modules within mcnpx for net neutron production by neutrons in the energy range 20 to 150 MeV. Similarly, the difference of 3.269 n/p in the values for net (n,xn) production is the value predicted by the new 150-MeV Pb data libraries for net neutron production by neutrons with energies between 20 and 150 MeV.

Case 2

In the second variation, we transport not only nucleons (denoted by the symbols n and h on the mode card) and charged pions (/), but also light ions (deuterons, tritons, 3He, and alphas, denoted by d, t, s, and a, respectively). The only differences between the two input decks are the two cards:

Base Case:
```
mode n h /
imp:n,h,/ 1 1r 0
```
Case 2:
```
mode n h / d t s a
imp:n,h,/,d,t,s,a 1 1r 0
```

Note that nuclear interactions by light ions are simulated using the ISABEL INC model. The problem summary for this case is shown below:

```
sample problem: spallation target: Case 2
neutron creation       tracks   weight        energy            neutron loss           tracks   weight        energy
                                 (per source particle)                                            (per source particle)

 source                     0    0.            0.                  escape              366756    1.8321E+01    2.1938E+02
 nucl. interaction     316952    1.5848E+01    3.2187E+02          energy cutoff            0    0.            0.
 particle decay             0    0.            0.                  time cutoff              0    0.            0.
 weight window              0    0.            0.                  weight window            0    0.            0.
 cell importance            0    0.            0.                  cell importance          0    0.            0.
 weight cutoff              0    0.            0.                  weight cutoff            0    0.            0.
 energy importance          0    0.            0.                  energy importance        0    0.            0.
 dxtran                     0    0.            0.                  dxtran                   0    0.            0.
 forced collisions          0    0.            0.                  forced collisions        0    0.            0.
 exp. transform             0    0.            0.                  exp. transform           0    0.            0.
 upscattering               0    0.            0.                  downscattering           0    0.            9.8368E+00
 tabular sampling           0    0.            0.                  capture                  0    1.4534E-02    7.7278E-02
 (n,xn)                 79010    3.9467E+00    1.9031E+01          loss to (n,xn)       25539    1.2753E+00    4.9548E+01
 fission                    0    0.            0.                  loss to fission          0    0.            0.
 photonuclear               0    0.            0.                  nucl. interaction     3667    1.8335E-01    6.2061E+01
 tabular boundary         0    0.            0.                  tabular boundary         0    0.            0.
 (gamma,xn)               0    0.            0.                  particle decay           0    0.            0.
 adjoint splitting        0    0.            0.
     total           395962    1.9794E+01    3.4090E+02              total           395962    1.9794E+01    3.4090E+02

  number of neutrons banked                   370423        average time of (shakes)              cutoffs
  neutron tracks per source particle      1.9798E+01          escape            5.7616E+00          tco   1.0000E+34
  neutron collisions per source particle  2.7981E+01          capture           4.8708E-01          eco   0.0000E+00
  total neutron collisions                    559626          capture or escape 5.7574E+00          wc1  -5.0000E-01
  net multiplication              0.0000E+00  .0000           any termination   5.3337E+00          wc2  -2.5000E-01
```

Calculated net neutron production for this case is 18.335, and examination of the net nuclear interactions and net (n,xn) figures show very similar results to the base case. The implication of this result is that we need not concern ourselves with light ion transport if the quantity with which we concerned is related solely to neutrons, as neutron production by light ions is small when we start with a proton beam.

Case 3

In this variation, we replace the Bertini INC model used in the base case for the simulation of nucleon and pion interactions with nuclei by the ISABEL INC model (in this example, both INC models utilize the same GCCI level density model). We invoke the ISABEL INC model by including in the input deck the following card:

Base Case: lca `j j j`

Case 3: `lca j j 2`

This changes the value of the variable IEXISA (third value on the lca card) from its default value of 1 to 2. The neutron problem summary for this case follows:

```
sample problem: spallation target: Case 3

neutron creation       tracks   weight        energy             neutron loss           tracks   weight        energy
                                 (per source particle)                                            (per source particle)

 source                   0    0.            0.                  escape              351353    1.7552E+01    2.2257E+02
 nucl. interaction   302047    1.5102E+01    3.2679E+02          energy cutoff            0    0.            0.
 particle decay           0    0.            0.                  time cutoff              0    0.            0.
 weight window            0    0.            0.                  weight window            0    0.            0.
 cell importance          0    0.            0.                  cell importance          0    0.            0.
 weight cutoff            0    0.            0.                  weight cutoff            0    0.            0.
 energy importance        0    0.            0.                  energy importance        0    0.            0.
 dxtran                   0    0.            0.                  dxtran                   0    0.            0.
 forced collisions        0    0.            0.                  forced collisions        0    0.            0.
 exp. transform           0    0.            0.                  exp. transform           0    0.            0.
 upscattering             0    0.            0.                  downscattering           0    0.            9.3603E+00
 tabular sampling         0    0.            0.                  capture                  0    1.3946E-02    7.4771E-02
 (n,xn)               78250    3.9089E+00    1.8916E+01          loss to (n,xn)       25121    1.2545E+00    4.9306E+01
 fission                  0    0.            0.                  loss to fission          0    0.            0.
 photonuclear             0    0.            0.                  nucl. interaction     3823    1.9115E-01    6.4394E+01
 tabular boundary         1    5.0000E-05    7.4505E-03          tabular boundary         1    5.0000E-05    7.4505E-03
 (gamma,xn)               0    0.            0.                  particle decay           0    0.            0.
 adjoint splitting        0    0.            0.
     total           380298    1.9011E+01    3.4571E+02              total           380298    1.9011E+01    3.4571E+02

  number of neutrons banked                   355177        average time of (shakes)              cutoffs
  neutron tracks per source particle      1.9015E+01          escape            5.7572E+00          tco   1.0000E+34
  neutron collisions per source particle  2.6865E+01          capture           4.9166E-01          eco   0.0000E+00
  total neutron collisions                    537297          capture or escape 5.7530E+00          wc1  -5.0000E-01
  net multiplication              0.0000E+00  .0000           any termination   5.3162E+00          wc2  -2.5000E-01
```

Note the net neutron production calculated with the ISABEL INC model is 17.569, which is 3.8% below the value predicted by the Bertini INC model. This is consistent with other studies that reveal slightly lower neutron production resulting from ISABEL as compared to Bertini.

Case 4

In the next variation from the base case we use the new evaluated proton libraries for transporting protons below 150 MeV, replacing the Bertini model used at all proton energies in the base case. We invoke transport of protons with energies less than 150 MeV by including a phys:h card to specify the transition energy between LAHET physics and data evaluations for proton transport:

Base Case: `phys:h 1000. j 0.`
Case 4: `phys:h 1000. j 150.`

The neutron summary table for this case is shown below.

```
sample problem: spallation target: Case 4


neutron creation       tracks   weight        energy            neutron loss           tracks   weight        energy
                                 (per source particle)                                           (per source particle)

 source                   0    0.            0.                  escape              365199    1.8244E+01    2.1884E+02
 nucl. interaction   308299    1.5415E+01    3.2024E+02          energy cutoff            0    0.            0.
 particle decay           0    0.            0.                  time cutoff              0    0.            0.
 weight window            0    0.            0.                  weight window            0    0.            0.
 cell importance          0    0.            0.                  cell importance          0    0.            0.
 weight cutoff            0    0.            0.                  weight cutoff            0    0.            0.
 energy importance        0    0.            0.                  energy importance        0    0.            0.
 dxtran                   0    0.            0.                  dxtran                   0    0.            0.
 forced collisions        0    0.            0.                  forced collisions        0    0.            0.
 exp. transform           0    0.            0.                  exp. transform           0    0.            0.
 upscattering             0    0.            0.                  downscattering           0    0.            9.8423E+00
 tabular sampling      7166    3.5830E-01    1.8289E+00          capture                  0    1.4179E-02    7.6277E-02
 (n,xn)               78791    3.9358E+00    1.9090E+01          loss to (n,xn)       25324    1.2646E+00    4.9542E+01
 fission                  0    0.            0.                  loss to fission          0    0.            0.
 photonuclear             0    0.            0.                  nucl. interaction     3733    1.8665E-01    6.2865E+01
 tabular boundary         0    0.            0.                  tabular boundary         0    0.            0.
 (gamma,xn)               0    0.            0.                  particle decay           0    0.            0.
 adjoint splitting        0    0.            0.
     total           394256    1.9709E+01    3.4116E+02              total           394256    1.9709E+01    3.4116E+02

  number of neutrons banked                   368932        average time of (shakes)              cutoffs
  neutron tracks per source particle      1.9713E+01          escape            5.7563E+00          tco   1.0000E+34
  neutron collisions per source particle  2.7817E+01          capture           4.6071E-01          eco   0.0000E+00
  total neutron collisions                    556332          capture or escape 5.7522E+00          wc1  -5.0000E-01
  net multiplication               0.0000E+00  .0000          any termination   5.3292E+00          wc2  -2.5000E-01
```

Net neutron production for this case is 18.285 n/p, which is 0.1% greater than the base case value. Thus, as for neutrons, the new 150-MeV proton evaluations for lead predict higher neutron production by protons in the energy range 20 to 150 MeV than does the Bertini INC model. Since the proton evaluations are considered to be more accurate than the Bertini model, the n/p value for this case should be considered more accurate than the value calculated in the base case.

Case 5

In the final variation from the base case we use the CEM model for neutron, protons and pions. CEM is turned on by setting the 9th entry of the LCA card to 1:

Base Case: `LCA j j j`
Case 4: `LCA j j j j j j j j 1`

The neutron summary table for this case is shown below.

```
sample problem: spallation target: Case 5

n creation       tracks   weight        energy            neutron loss           tracks   weight        energy

                                 (per source particle)                                           (per source particle)


 source                   0    0.            0.                  escape               313015    1.5635E+01    2.1374E+02
 nucl. interaction   254437    1.2722E+01    3.1302E+02          energy cutoff             0    0.            0.
 particle decay           0    0.            0.                  time cutoff               0    0.            0.
 weight window            0    0.            0.                  weight window             0    0.            0.
 cell importance          0    0.            0.                  cell importance           0    0.            0.
 weight cutoff            0    0.            0.                  weight cutoff             0    0.            0.
 energy importance        0    0.            0.                  energy importance         0    0.            0.
 dxtran                   0    0.            0.                  dxtran                    0    0.            0.
 forced collisions        0    0.            0.                  forced collisions         0    0.            0.
 exp. transform           0    0.            0.                  exp. transform            0    0.            0.
 upscattering             0    0.            0.                  downscattering            0    0.            7.3438E+00
 tabular sampling         0    0.            0.                  capture                   0    1.3051E-02    8.5469E-02
 (n,xn)               91571    4.5738E+00    2.1850E+01          loss to (n,xn)        29374    1.4667E+00    5.7124E+01
 fission                  0    0.            0.                  loss to fission           0    0.            0.
 photonuclear             0    0.            0.                  nucl. interaction      3619    1.8095E-01    5.6576E+01
 tabular boundary         1    5.0000E-05    7.4680E-03          tabular boundary          1    5.0000E-05    7.4680E-03
 (gamma,xn)               0    0.            0.                  particle decay            0    0.            0.
 adjoint splitting        0    0.            0.
     total           346009    1.7296E+01    3.3488E+02              total            346009    1.7296E+01    3.3488E+02

  number of neutrons banked                   316635        average time of (shakes)              cutoffs
  neutron tracks per source particle      1.7300E+01          escape            5.7337E+00          tco   1.0000E+34
  neutron collisions per source particle  2.3611E+01          capture           4.7022E-01          eco   0.0000E+00
  total neutron collisions                    472212          capture or escape 5.7293E+00          wc1  -5.0000E-01
  net multiplication               0.0000E+00  .0000          any termination   5.1842E+00          wc2  -2.5000E-01
```

Net neutron production for this case is 15.648 n/p, which is 14.3% than the base case value. Note also that CEM took twice as long to run as the base case. Both of these factors are well known, and CEM improvements is a very active project in the MCNPX program. The increase in time is understood, and will be corrected in future versions through algorithm optimization. The lower n/p values are also being extensively benchmarked, and improvements involving the transitions from INC to Preequilibrium, and Preequilibrium to evaporation have been developed. Until the new version is available, the user should be cautious in using the CEM model for production calculations.

Summary

Results compiled for each case of this example are shown in Table A-2. Note the run time for the case where the ISABEL INC model is used is about 15% greater than the base case using the Bertini model. Case 2 also runs slower since the light ion interactions are provided by the ISABEL model. Invoking the 150-MeV proton libraries slows execution by about 11% in this example.

Table A-2. Results Compiled for Summary Cases

Case	Variation from base case	Runtime (minutes)[a]	n/p
base	n/a	27.66	18.263
1	LAHET transport for 20-150 MeV neutrons	28.44	18.364
2	light ion transport & nuclear inter-action	33.55	18.335
3	ISABEL INC for nucleons and pions	31.91	17.569
4	evaluated data used for protons below 150 MeV	30.66	18.285
5	CEM INC for nucleons and pions	60.14	15.638

[a] Cases were run on an IBM AIX box.

This example demonstrates how to calculate neutron production from a spallation target. Use of the new LA150 library that extends evaluated nuclear data up to 150 MeV gives the most accurate results, particularly if the new proton evaluations are used in addition to the neutron evaluations. When the quantity of interest depends only on neutrons and one starts with a proton beam, there is no need to transport any particles other than protons, neutrons, and charged pions, as neutron production by other particles is negligible compared to production by these three particle types[1]. Use of the various LAHET physics model options, such as the ISABEL and CEM INC modules, within MCNPX is encouraged—this provides the user with the ability to test the sensitivity of the quantity of interest to the different physics models. If significant differences are observed, the user should evaluate which physics model is most appropriate for his or her particular application. For example, total neutron production from actinide targets is known to be more accurate if the multi-step preequilibrium model (MPM) is turned off, which is not its default setting.

[1] All particles should be included for energy deposition calculations, as discussed in Section 8.3.

Appendix B – HTAPE3X for use with MCNPX

This appendix is reprinted from "HTAPE3X for Use with MCNPX," Richard E. Prael, Los Alamos Report LA-UR-99-1992, April 16, 1999.

Abstract

HTAPE3X is a code for processing medium- and high-energy collision data written to a history file by MCNPX. In addition, it provides surface flux and current edits which supplement the standard MCNP tallies.

1. The HTAPE3X Code

HTAPE3X is a modification of the HTAPE code from the LAHET Code System [1] designed to provide analysis of the history file HISTP optionally written by MCNPX [2]. It is primarily intended to provide an analysis of the outcome of collisions in the medium- and high-energy range where the interaction physics is obtained from LAHET.

However, all appropriate features have been retained, even when they duplicate existing MCNP flux and current tallies [3]. The latter features relate to editing a "surface source write (SSW)" file (default name WSSA). For experienced LAHET users, they do provide some options not available with standard MCNP F1 and F2 tallies.

Note that the information written to HISTP comes only from interactions processed by the medium- and high-energy modules in MCNPX; low-energy neutron and proton (and any photon/electron) collisions which utilize MCNP library data do not contribute to the collision information on the history file and will not contribute to edits by HTAPE3X of collision data. Surface crossing edits from data on the file WSSA will apply to all particle types and all energies.

2. Input for HTAPE3X

The input structure is largely unchanged from the description in reference [1]. In general, energy units are MeV, time units are nanoseconds, and length units are centimeters. Note the difference in the time scale from MCNP practice.

The input file (default name INT) for HTAPE3X 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" [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 an "S" 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,ITMULT/

Some of the parameters in this record may optionally be preceded by a minus sign whose meaning is defined below (see Table D2 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.

Table B-1. Applicability of Input Control Parameters

IOPT	NERG	NTIM	NTYPE	NPARM	NFPRM	KPLOT	IXOUT	IMERGE	ITCONV	IRSP	ITMULT
1	O	O	R	R	O	N	N	O	O	O	O
101	O	O	R	R	O	N	N	O	O	O	O
2, 102	O	O	R	R	N	N	N	O	O	O	O
3	O	O	N	0	N	0	N	N	0	N	N
103	O	O	N	R	N	0	N	N	0	N	N
5	N	N	N	0	N	0	N	N	N	N	N
105	N	N	N	R	N	0	N	N	N	N	N
8	N	N	N	0	N	0	0	N	N	N	N
108	N	N	N	R	N	0	0	N	N	N	N
9, 109	O	O	R	R	O	N	N	O	O	O	O
10, 110	O	O	R	R	N	N	N	O	O	O	O
11, 111	O	N	R	R	O	N	N	O	N	N	N
12, 112	O	N	R	R	O	N	N	O	N	N	N
13	O	O	R	O	O	N	N	O	O	O	O
14	N	N	N	O	N	N	N	N	N	N	O

Table B-1. Applicability of Input Control Parameters (Continued)

IOPT	NERG	NTIM	NTYPE	NPARM	NFPRM	KPLOT	IXOUT	IMERGE	ITCONV	IRSP	ITMULT
114	N	N	N	R	N	N	N	N	N	N	O
15	N	N	N	O	N	O	O	N	N	N	N
115	N	N	N	R	N	O	O	N	N	N	N
16	O	N	N	0	N	O	N	N	N	N	N
116	O	N	N	R	N	O	N	N	N	N	N

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

IOPT defines the editing option to be applied as defined below. For all but IOPT = 13, 100 may added 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.

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 > I 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.

Table B-2. Applicability of Minus-Sign Flags on Input Control Parameters

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
5, 105	O	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

Table B-2. Applicability of Minus-Sign Flags on Input Control Parameters (Continued)

IOPT	-IOPT	-NERG	-NTIM	-NTYPE	-NPARM	-NFPRM
15, 115	O	N	N	N	O	N
116	O	O	N	N	O	N

O ≡ optional; N ≡ not used.

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+ I normalization divisors will be read in as described below. *The default is 0*; however, some options require that a value be supplied.

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*.

Table B-3. Particle Type Identification in HTAPE3X

Type	LAHET Usage	MCNPX Usage
0	proton	proton, $\bar{p}$
1	neutron	neutron, $\bar{n}$
2	π^+	π^+, π^-
3	π^0	π^0
4	π^-	
5	μ^+	

Table B-3. Particle Type Identification in HTAPE3X (Continued)

Type	LAHET Usage	MCNPX Usage
6	μ^-	μ^-, μ^+
7	deuteron	deuteron
8	triton	triton
9	^{3}He	^{3}He
10	alpha	alpha
11	photon	photon
12	K^+	K^+, K^-
13	K^0long	K^0long
14	K^0short	K^0short
15	K^-	
16	$\bar{p}$	
17	$\bar{n}$	
18	electron	electron, positron
19	positron	
20	neutrino	neutrino, antineutrino
21	antineutrino	

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 (provided it has been installed with the code using the LANL CGS and CGSHIGH Common Graphics System libraries). 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 19 below).

IMERGE is not used in HTAPE3X; see Section 20 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 21 below).

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 22 below.

ITMULT is the TIME MULTIPLIER flag. ITMULT > 0 indicates that the weights tallied will be *multiplied* by the event time. This option applies only when the basic option type is 1, 2, 4, 9, 10, or 13.

The standard definitions for these input variables may not apply for some options. The applicability of the option control parameters is summarized in Table D1.

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.

Table B-4. Order of HTAPE3X Input Records

(-)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-1	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

- For NTYPE > 0, a record containing NTYPE particle types in any order, defined as the array ITIP(I),I=I,NTYPE. In the present MCNPX version 2.3.0, the contents of a surface source file WSSA are insufficient to distinguish between a particle and its antiparticle; it is to be expected that this condition will be remedied in future releases of MCNPX. The allowed particle types are listed in Table D3, which also indicates the overlapping particle/antiparticle tally definition which follows the column "MCNPX Usage."
- For NPARM > 0, a record containing NPARM *user-defined* cell, material, or surface numbers (integers), in any order, for which one wishes a tally to be made; these are defined as the array LPARM(I),I=1,NPARM. If a null record ("/") is supplied with NPARM > 0, it is treated as "1,2,3,...NPARM/". (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 HTAPE3X 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 2.4 of reference [1]) followed by the new source definition record (also in LAHET format).
- For ITCONV ≠ 0, a LAHET source time distribution record as described in Section 2.4 of reference [1].
- For IRSP ≠ 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 < 200 is obtained from the array ERESP input (terminated by a "/”). The user must maintain the proper correspondence among the arrays (see Section 22 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 D4.

3. Edit Option 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. 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. 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, all 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.

Segmenting may also be accomplished by using segmenting cylinders. The input has the same format as segmenting by planes; however, IFSEG negative designates cylindrical segmenting. IFSEG = -1 indicates that the segmenting cylinders are concentric with the x-axis; IFSEG = -2 indicates that the segmenting cylinders are concentric with the y-axis; IFSEG = -3 indicates that the segmenting cylinders are concentric with the z-axis. The values of the FSEG array are the radii of nested concentric cylinders and must be in increasing order. Segmenting cylinders are concentric with an axis, not just parallel.

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.

4. Edit Option IOPT = 2 or 102 : Surface Flux

The surface flux tally is analogous to an MCNP F2 tally. 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 I above; the same input record to designate the segmenting planes or cylinders 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.

5. Edit Option 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 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 particle 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.

6. Edit Option IOPT = 4 or 104 : Track Length Estimate for Neutron Flux

Option 4 is not available in this version; use a standard F4 flux tally.

7. Edit Option 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. Only nonelastic interactions are included. The option accesses the 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.

8. Edit Option IOPT = 6 or 106 Energy Deposition

Option 6 is not available in this version.

9. Edit Option IOPT = 7 : Mass and Energy Balance

Option 7 is not available in this version.

10. Edit Option 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 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, including elastic collisions. 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, NTYPE, and NFPRM are unused. If IXOUT = 1, an auxiliary output file appropriate for input to the CINDER program will be written; the default file name is OPT8A. Unless otherwise modified, tally units are dimensionless (weight of a residual nuclide per source particle).

An additional tabulation is produced which shows the estimated metastable state production as a fraction of the total isotopic production. As illustrated in the example here, a state is identified by its excitation energy and half-life; the estimated fraction of total isotope production associated with the particular metastable state is shown with the estimated relative standard deviation.

z	a	elev	t-half	fraction
*				
*				
47	110	0.11770	2.17730D+07	4.00000D-01 0.3465
47	111	0.05990	6.50000D+01	8.00000D-01 0.2001
47	116	0.08100	1.05000D+01	S.00000D-01 0.5001
48	113	0.26370	4.41500D+08	2.85714D-01 0.3195
48	115	0.17340	3.87070D+06	5.00000D-01 0.3536
48	117	0.13000	1.22400D+04	2.50000D-01 0.4331
48	119	0.14640	1.62000D+02	6.00000D-01 0.2329

11. Edit Option 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. 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/

12. Edit Option 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. 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.

13. Edit Option 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 *t* of crossing in the bin, the standard deviation σ of $\bar{t}$ given by $(t^2 - \bar{t}^2)$ ½, the figure of merit FOM1 given by (current)/σ^2 and the figure of merit FOM2 given by (current)/σ^3.

Unless otherwise modified, the current tally is dimensionless. The units of $\bar{t}$ and σ are nanoseconds, while FOM1 is in ns^{-2} and FOM2 is in ns^{-3}. The parameter FNORM is used to adjust the units of the time variable, which are nanoseconds in LAHET3, 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.

14. Edit Option 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." The input is identical to option 9, with the exception that NTIM is unused.

15. Edit Option IOPT = 13 : Global Emission Spectrum

The original definition [l] of option 13 was given by

> 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.

Surface crossing records appearing on a SSW-written file are not distinguished as to whether they correspond to an internal surface crossing or to escape into the external void. Therefore, for use with MCNPX, the original intent of this option may most easily be achieved by defining the external importance 0 (leakage) region as the exterior of a sphere containing the complete geometry; then only specifying the defining spherical surface on the SSW card that controls the contents of the surface crossing file.

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 are 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 ø 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 D-1. The allowed options are as follows:

> KOPT = 1: the +z-axis defines the polar angle and ø is measured counter-clockwise from the +x-direction;
>
> KOPT = 2: the +z-axis defines the polar angle and ø is measured counter-clockwise from the +y-direction;
>
> KOPT = 3: the +x-axis defines the polar angle and ø is measured counter-clockwise from the +y-direction;
>
> KOPT = 4: the +x-axis defines the polar angle and ø is measured count er- clockwise from the +z-direction;

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

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

A value of KOPT = 0 defaults to KOPT = 1. For NPARM ≥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.

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/ ,
-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. 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.

16. Edit Option IOPT = 14 or 114 : Gas Production

Option 14 provides an edit of hydrogen and helium gas production, by isotope, by element, and total. 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. The estimate is made by tallying all H and He ions stopped in a cell or material, including source particles.

17. Edit Option IOPT = 15 or 115 : Isotopic Collision Rate

Option 15 has been added to provide a collision rate edit by target isotope. The input has the same meaning as for IOPT = 8, with the following exceptions: KOPT = 0 or 1 tabulates all collisions; KOPT = 2 or 3 tabulates elastic scattering only; KOPT = 4 or 5 tabulates non-elastic events only. If KOPT is even, the edit is by cell number; if KOPT is odd, the edit is by material number. A CINDER removal rate input file will produced for IXOUT > 0. The default CINDER file name is OPT15A.

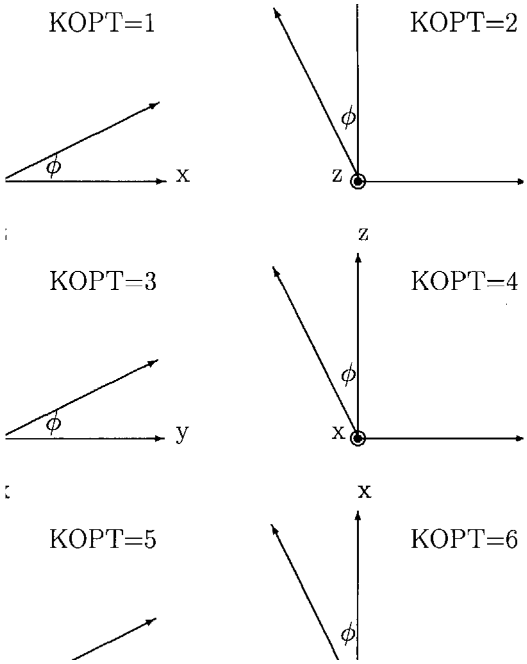

Figure B-1. Use of the KOPT Parameter for HTAPE3X Option 13.

18. Edit Option IOPT = 16 or 116 : Recoil Energy and Damage Energy Spectra

Option 16 provides an edit of the spectra of total recoil energy, elastic recoil energy, total damage energy, and elastic damage energy. Also estimated are the mean weight of recoiling fragments per history, mean weight of recoil (or damage) energy per history, and the mean energy per fragment (the ratio of the previous two estimates). NERG specifies the number of energy bins for the spectra; a minus sign on NERG will have the tabulation normed per MeV (recommended to produce a true spectrum). Input variables NTIM, NTYP, NFPRM, IXOUT, IRS, IMERGE, ITCONV, and IRSP are unused. KOPT = 0 indicates tally by cell; KOPT = 1 indicates tally by material. NPARM is the number of cells (or materials) to be read in for the tally. If a minus sign flag is used with IOPT (IOPT = -16), the weights tallied for the spectra will be multiplied by corresponding recoil (or damage) energy.

At any collision, the damage energy E_d is obtained from the recoil energy E_r of nucleus A_r, Z_r by the relation of Linhard [4]

$$E_d = E_r\, L\, (E_r)$$

using the formulation of Robinson [5]:

$$k_i = \frac{0.133745 Z_r^{2/3} Z_i^{1/2}}{A_r^{3/2} A_i} \left(\frac{A_r + A_i}{2}\right)^2 \left(\frac{2}{Z_r^{2/3} + Z_i^{2/3}}\right)^{3/4}$$

$$\epsilon_i = \frac{0.03252 A_i E_r}{(A_r + A_i) Z_r Z_i (Z_r^{2/3} + Z_i^{2/3})^{1/2}}$$

$$g(\epsilon_i) = \epsilon_i + 0.40244 \epsilon_i^{3/4} + 3.4008 \epsilon_i^{1/6}$$

$$L(E_r) = \sum_{i=1}^{n} \frac{f_i}{1 + k_i g(\epsilon_i)}$$

where the summation is over the components of the material with atom fractions f_i.

19. 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 calculation. For its application, see reference [1].

20. The Merge Option

Not used in HTAPE3X. For any tally *either* the HISTP file *or* the HISTX file is edited, but not both.

21. The Time Convolution Option

Assume that an initial calculation has been made with the default source time distribution (i.e., all histories start at t=O). A time-dependent tally for *any* of the allowed LAHET source time distributions may then be made with HTAPE3X without rerunning the transport calculation. For details, see reference [1].

22. 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 2 above. 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 ≤ ERESP(I+1). For IRSP > 0, the interpolated response function value *multiplies* the tally increment; for IRSP < 07 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.

23. Executing HTAPE3X

The default file name for the input is INT; the default file name for the output is OUTT; the default file name for the history file is HISTP; and the default file name for the surface crossing file is HISTX for input into HTAPE3X. (The latter is written by MCNPX with the default file name WSSA.) If option 8 is requested, the data file PHTLIB must be in the user's file space; if option 16 is requested, the data file BERTIN must be in the user's file space. All these file names may be defined by file replacement on the execute line:

```
HTAPE3X INT=my_input OUTT=my_output HISTP=file1 HISTX=file2
```

References

[1] R. E. Prael and H. 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

[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] J. F. Briesmeister, editor, *MCNP™—A General Monte Carlo N-Particle Transport Code*, Los Alamos National Laboratory report LA-12625-M (March 1997). http://www-xdiv.lanl.gov/XCI/PROJECTS/MCNP/manual.html

[4] J. Linhard, V. Nielsen, and M. Scharff, *Kgl. Dan. Vidensk. Selsk., Mat.-Fys. Medd*. 36, No. 10 (1968).

[5] M. Robinson, "The Dependence of Radiation Effects on Primary Recoil Energy," *Radiation Induced Voids in Metals*, AEC Symp. Ser. 26, p. 397, US Atomic Energy Commission (1971).

Appendix C – Using XSEX3 with MCNP

1. Introduction

XSEX3 is the code which analyzes a history file produced by LAHET3 or MCNPX and generates double-differential particle production cross sections for primary beam interactions. Cross section plots may also be generated by creating a file to be plotted by MCNP. It is necessary to execute either code in a specific mode, described below, to achieve the desired cross section calculation.

The execution of XSEX3 assumes that the LAHET run was made using the option **N1COL** = -1. Under this 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. The procedure may be used to calculate double-differential particle production cross sections from any of the interaction models in the code (Bertini, ISABEL, CEM, etc.); the procedure has no meaning if such a model is not allowed for the specified particle type at the specified energy.

2. Input for MCNPX

Since there is no way to avoid the MCNPX 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. Note: with **N1COL** = -1, MCNPX will override the source specification and construct the source as a ``pencil-beam'' in the +z-direction as required by XSEX3. Other MCNPX options may be used to suppress either nuclear elastic or nonelastic reactions.

1. To create a HISTP file to be edited by XSEX3, include a HISTP card in the INP file.
2. Define a volume parallel beam source in the +z-direction (vec = 0 0 1) which is completely contained inside a cell with the material for which the cross sections are to be calculated.
3. Specify the incident particle type and kinetic energy on the SDEF card.
4. Use **NOACT**=1 (the 8th parameter) on the LCA card.

The user may wish to suppress nuclear elastic scattering in the calculation by using **IELAS**=0 on the **LCA** card. An **AWTAB** card may need to be supplied if the target isotope has no mass in XSDIR; the value supplied is not used and is arbitrary.

As an example, the following is a sample MCNPX input for a cross section calculation:

```
MCNPX standard cross section generation format for XSEX3 use.
c ------------------------------------------------------------------
c 1000 MeV protons on Sn121, an isotope not in MCNP library,
c and for which no atomic weight is specified in XSDIR.
c Minimal geometric specification for this purpose.
c ------------------------------------------------------------------
c Cell - only one, spherical, radius arbitrary
c ------------------------------------------------------------------
 1  1 -1.0  -1
 2  0       1

c ------------------------------------------------------------------
c Surface - one sphere, radius arbitrary
c ------------------------------------------------------------------
 1  so  50.0

c ------------------------------------------------------------------
c Materials
c ------------------------------------------------------------------
  m1    50121 1       $ not in MCNP libraries
  awtab 50121 119.864 $ need value, but arbitrary
c ------------------------------------------------------------------
c Source - 0 radius beam, +z-direction, 1 GeV proton
c ------------------------------------------------------------------
  sdef erg = 1000 par = 9 dir = 1 pos = 0 0 0 rad = 0.0 vec = 0 0 1
c ------------------------------------------------------------------
c Options - no elastic, Bertini, energy balancing
c ------------------------------------------------------------------
  lca   0 6j -1
  lea   2j 0
c ------------------------------------------------------------------
c History file - "histp" required
c ------------------------------------------------------------------
  histp
c ------------------------------------------------------------------
c Tallies - none
c ------------------------------------------------------------------
  imp:h 1 0
  phys:h 1000
  mode h
  print
  nps 1000
  prdmp 2j -1
```

3. Input for XSEX3

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

1. Two records of title information, 80 columns each
2. An option control record (list-directed format)
3. 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,IMOM,IYIELD,LTEST

Parameter	Meaning
NERG	Defines the number of energy or momentum bins for which cross sections will be calculated. For NERG \GT 0, an energy (momentum) boundary record is required. For NERG = 0, only energy-integrated cross sections will be generated. The default is 0.
NANG	Defines the number of cosine bins for which cross sections will be calculated. For NANG not equal to 0, a angular boundary record is required. For NANG = 0, only angle-integrated cross sections will be generated. Positive values of NANG indicate cosine bin boundaries will be defined; negative values indicate angle bin boundaries (in degrees!) will be specified. The default is 0.
FNORM	An overall multiplicative normalization factor to be applied to all cross sections. The default is 1.0. To convert to millibarns, use FNORM = 1000; o obtain macroscopic cross sections, use an atom density.
KPLOT	A plot control flag; the default is 0. Any nonzero value will cause the output to be written to a file XSTAL in the format of an MCNP MCTAL file for subsequent plotting (see below.)

Parameter	Meaning
IMOM	Chooses energy or momentum to be used in cross section definition. IMOM = 0, cross sections are tabulated by energy (MeV) and differential cross sections are calculated per unit energy (per MeV). IMOM not equal 0, cross sections are tabulated by momentum (MeV/c) and differential cross sections are estimated per unit momentum (per MeV/c).
IYIELD	not equal to 0 estimates differential yields (or multiplicities) for nonelastic and elastic reactions rather than cross sections. The integral over energy and angle for each particle type will be the multiplicity per nonelastic reaction (or unity for the elastic scattering of the incident particle if it is included in the calculation).
LTEST	not equal to 0 suppresses date and timing on the conventional output file (OUTXS). the default is 0. LTEST is used to produce output for comparison during MCNPX installation and should not be used generally.

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

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:

1. The energy boundary array may be fully entered as ERGB(I), I=1,NERG, in increasing order.
2. 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.
3. If only one entry is given, it is used as the first upper energy boundary and also as a constant spacing between all the boundaries.
4. 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 ``{\bf -0.1,800./}'' will specify ten equal-lethargy bins per decade from 800 MeV down.

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.

For NANG < 0, a record is required to define the \BAR NANG \BAR lower degree bin boundaries. They should be entered from low to high, with the last lower boundary equal to 0.0; the upper limit of the first bin is always 180 degrees. If a null record is present (only a ``/''),then the range (180,0) is divided into \BAR NANG \BAR equal intervals.

4. Executing XSEX3

An input file and a history file are the only required input files. 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. A value of KPLOT \NE 0 will result in the creation of a MCTAL-format plot file, with default name XSTAL. These file names may be changed by file replacement. The most general execute line has the format:

XSEX3 INXS=... OUTXS=... HISTP=... XSTAL=...

4. Plotting Output from XSEX3

The source code for XSEX3 contains a plotting package using the LANL Common Graphics System; the latter is not generally available outside of Los Alamos National Laboratory. A new feature has been added for this release whereby a nonzero value for the input quantity KPLOT will cause the writing of a file XSTAL in the format of an MCNPX MCTAL file. Plotting of XSTAL is performed by MCNPX, using the execution option

mcnpx z

followed by the required instructions

rmctal xstal
nonorm

The latter is essential since the data are normalized in XSEX3.

Each “case” in XSEX3 is expanded in the XSTAL file for each particle type produced. The tallies are identified by the numbering scheme

100(case number) + (particle type),

the latter defined in the table below. The last in the sequence corresponds to the elastic scattering distribution of the incident particle.

When plotting XSEX3 output, the appropriate y-axis labels are ``barns/MeV/steradian'', ``barns/MeV'' or ``barns/steradian''. If the ``yield'' (multiplicity) option was used in XSEX3, the appropriate y-axis labels are ``particles/MeV/steradian'', etc. The energy axis may be either ``energy (MeV)'' or ``momentum (MeV/c)'' according to the XSEX3 option employed.

Type	Particle
1	proton
2	neutron
3	pi+
4	pi0
5	pi-
6	deuteron
7	triton
8	He-3
9	alpha
10	photon (prompt gamma from residual)
11	K+
12	K (all neutrals)
13	K-
14	antiproton
15	antineutron
16	elastic scattered projectile

An example of a COMOUT file produced when plotting XSTAL is shown on the next page.

```
rmctal xstala
nonorm
tally 101 free e loglog xlims 0.1 1000. ytitle "protons/MeV" file
free c linlog xlims -1.0 +1.0 ytitle "protons/steradian" file
tally 102 free e loglog xlims 0.1 1000. ytitle "neutrons/MeV" file
free c linlog xlims -1.0 +1.0 ytitle "neutrons/steradian" file
tally 103 free e loglog xlims 0.1 1000. ytitle "pi+/MeV" file
free c linlog xlims -1.0 +1.0 ytitle "pi+/steradian" file
tally 104 free e loglog xlims 0.1 1000. ytitle "pi0/MeV" file
free c linlog xlims -1.0 +1.0 ytitle "pi0/steradian" file
tally 105 free e loglog xlims 0.1 1000. ytitle "pi-/MeV" file
free c linlog xlims -1.0 +1.0 ytitle "pi-/steradian" file
tally 106 free e loglog xlims 0.1 1000. ytitle "deuterons/MeV" file
free c linlog xlims -1.0 +1.0 ytitle "deuterons/steradian" file
tally 107 free e loglog xlims 0.1 1000. ytitle "tritons/MeV" file
free c linlog xlims -1.0 +1.0 ytitle "tritons/steradian" file
tally 108 free e loglog xlims 0.1 1000. ytitle "He-3/MeV" file
free c linlog xlims -1.0 +1.0 ytitle "He-3/steradian" file
tally 109 free e loglog xlims 0.1 1000. ytitle "alphas/MeV" file
free c linlog xlims -1.0 +1.0 ytitle "alphas/steradian" file
tally 110 free e loglog xlims 0.1 100. ytitle "photons/MeV" file
free c linlog xlims -1.0 +1.0 ytitle "photons/steradian" file
end
```