LA-UR 95-2129

CONF-9509100--20

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

TITLE: MCNP™ CRITICALITY PRIMER AND TRAINING EXPERIENCES

AUTHOR(S): J. Briesmeister
A. Forster

R. Busch, UNM

DISCLAIMER

SUBMITTED TO: The Fifth International Conference on Nuclear Criticality Safety, Albuquerque, New Mexico, September 17-21, 1995.

Los Alamos
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

FORM NO 836 R4

MCNP™ CRITICALITY PRIMER AND TRAINING EXPERIENCES

Judith Briesmeister and R. Arthur Forster
University of California
Los Alamos National Laboratory
Los Alamos New Mexico 87545
(505) 667-7277 , FAX (505) 665-5538
jfb@lanl.gov

Robert Busch
Chemical and Nuclear Engineering Department
University of New Mexico
Albuquerque, New Mexico 87131-1341
(505) 277-8027, FAX (505) 277-5433
busch@unm.edu

INTRODUCTION

With the closure of many experimental facilities, the nuclear criticality safety analyst is increasingly required to rely on computer calculations to identify safe limits for the handling and storage of fissile materials. However, the analyst may have little experience with the specific codes available at his or her facility. Usually, the codes are quite complex, black boxes capable of analyzing numerous problems with a myriad of input options. Documentation for these codes is designed to cover all the possible configurations and types of analyses but does not give much detail on any particular type of analysis. For criticality calculations, the user of a code is primarily interested in the value of the effective multiplication factor for a system (k_{eff}). Most codes will provide this, and truckloads of other information that may be less pertinent to criticality calculations.

Based on discussions with code users in the nuclear criticality safety community, it was decided that a simple document discussing the ins and outs of criticality calculations with specific codes would be quite useful. The Transport Methods Group, XTM, at Los Alamos National Laboratory (LANL) decided to develop a primer for criticality calculations with their Monte Carlo code, MCNP. This was a joint task between LANL with a knowledge and understanding of the nuances and capabilities of MCNP and the University of New Mexico with a knowledge and understanding of nuclear criticality safety calculations and educating first time users of neutronics calculations. The initial problem was that the MCNP manual[1] just contained too much information. Almost everything one needs to know about MCNP can be found in the manual; the problem is that there is more information than a user requires to do a simple k_{eff} calculation. The basic concept of the primer[2] was to distill the manual to create a document whose only focus was criticality calculations using MCNP.

PHILOSOPHY OF THE PRIMER

The primer is designed to help the criticality analyst understand and use the MCNP Monte Carlo code for nuclear criticality safety analyses. It assumes a college education in a technical field, but there is no assumption of familiarity with Monte Carlo codes in general or with MCNP in particular. The primer teaches by example, with each example illustrating two or three features of MCNP often used in criticality analyses.

The primer provides a starting point for the criticality analyst using MCNP. Although self contained, the primer is intended as a companion volume to the MCNP manual. Specific examples of using MCNP for criticality analyses are given in the primer while the manual gives information on the use of MCNP in all aspects of particle transport calculations. The primer also contains appendices that give the user a general description of Monte Carlo techniques, the default cross sections available in MCNP, surface descriptions, and other reference data. This information is provided in appendices so as not to obscure the basic information illustrated in each example.

Starting with a Quickstart chapter, the primer gives an overview of the basic requirements for MCNP input and allows the reader to quickly run a simple criticality problem with MCNP. This chapter is not designed to explain either the input or the MCNP options in detail, but to introduce basic concepts that are further explained in following chapters. Each chapter has a list of objectives at the beginning that identifies the focus of the chapter and the individual MCNP features covered in detail in the example problems of that chapter. It is expected that on completion of the primer, the reader will be comfortable using MCNP in criticality calculations and could handle 80 to 90% of the situations that normally arise in a facility. The primer provides a set of basic input files that can be selectively edited for use with any particular problem.

The primer is designed to be useful and easy to read. As with most manuals, the user gets the most out of it by starting with Chapter One and proceeding through the rest of the chapters in order. Each chapter assumes knowledge and comfort with the concepts discussed in the previous chapters. Although it may be tempting to pick up the primer and immediately go to the example problem that is similar to an analysis requirement, this approach will not give the user the background or the confidence in analysis ability necessary for safe implementation of procedures and limits. There is no substitute for a thorough understanding of the techniques used in an MCNP analysis. A little extra time spent going through the primer and doing the examples will save many hours of confusion and embarrassment later.

Primer Format

To make the primer easy to use, a standard set of notation was developed. The text is set in Times Roman type. Information that the user types into an input file is set in `Courier`. Characters in the Courier font represent commands, keywords, or data used as computer input. As the primer often references the MCNP manual, these references are set in square brackets, e.g., [see MCNP Manual Chapter x].

One novel feature of the primer is the use of what we called *grey boxes*. These present underlying philosophy and mini-tutorials on specific ideas or features of MCNP. As an example, we used a grey box to discuss 'The Universe Concept.' In MCNP, the use of universes can substantially reduce input for repeated structures and lattices so we used a grey box to introduce the concept of a universe.

The Universe Concept

A universe is either a lattice or an arbitrary collection of cells that, once defined, can be used to fill other cells within a geometry. Another way to think of it is to look out a window at the sky. You can see part of the sky but not all of it because of the window edges. There is essentially an infinite amount of sky but you are limited to what the window allows you to see. The window is the filled cell and the sky is the universe that fills the cell.

In this chapter the universe will be a collection of cells. In other words, several cells will be defined to be in a universe and another cell will be filled with that universe. (Lattices will be explained in later chapters of the primer.)

Recalling the card format from Chapter 1, the universe card is entered in the `params` section of the cell card. Universe numbers are arbitrary integers chosen by the user. There are two rules when using universes.

1. The cells of a universe can be finite or infinite but must completely fill all of the space within the cell that the universe is specified to fill.

2. The surfaces of a filled cell and surfaces of the filling universe must never coincide.

The 17 grey boxes are interspersed throughout the primer to provide quick tutorials on concepts specific to MCNP. In this way the reader can go directly to a grey box to get a refresher course on a particular topic.

Primer Contents

The primer begins with an introduction that describes its objectives and provides an overview of MCNP. This is followed by seven chapters arranged in a standard format. Each chapter starts with the objectives or 'what you will be able to do' after completing the chapter. Then one or more example problems based on real critical assemblies are used to highlight the MCNP topics discussed in detail in the chapter. After running these problems, the results are given followed by a summary of the material contained in the chapter. The seven chapters, their objectives, and the problem configurations associated with them are given in Table 1.

TABLE 1

CRITICALITY PRIMER CHAPTERS

CHAPTER 1: MCNP *QUICKSTART*

objectives - what the reader will be able to do:

interpret an MCNP input file

set up and run a simple criticality problem on MCNP

interpret k_{eff} information from MCNP output

Problem - Bare Pu Sphere (Jezebel)

CHAPTER 2: REFLECTED SYSTEMS

objectives - what the reader will be able to do:

interpret the sense of a surface

use the Boolean intersection, union, and complement geometry operators

define a multicell problem

Problem - Pu Metal Cylinder without and with natural U Reflectors

CHAPTER 3: S(α,β) THERMAL NEUTRON TREATMENT FOR MODERATORS

objectives - what the reader will be able to do:

use and understand use S(α,β) thermal neutron treatment

understand the order of geometry operations on cell cards

see effects of S(α,β) treatment

interpret k_{eff} output

Problem - Bare U(4.89) O_2F_2 Solution Cylinder

CHAPTER 4: SIMPLE REPEATED STRUCTURES

objectives - what the reader will be able to do:

use the universe (*u*) and *fill* cards

use the *like m but* card

use the *trcl* card

use the 2-D color geometry plotting capability

Problem - 2 U(93.4)O_2F_2 Cylinders inside a W[illegible]nk

CHAPTER 5: HEXAHEDRAL (SQUARE) LA[illegible]

objectives - what the reader will be able to do:

use the *lat* keyword to create a square lattice

understand lattice indexing

create a lattice whose elements: contain different materials, are filled with different sized items or are sometimes empty

Problem - 3x2 Array of Plutonium Nitrate Cylinders

CHAPTER 6: HEXAGONAL (TRIANGULAR) LATTICES

objectives - what the reader will be able to do:

create general planes to define a hexagonal lattice element

use the *lat* keyword to create a hexagonal (triangular pitch) lattice

understand hexagonal lattice indexing

Problem - Hexagonal Array of 7 U(93.2) O_2F_2 Cylinders with reflection

CHAPTER 7: 3-DIMENSION SQUARE LATTICES

objectives - what the reader will be able to do:

create a 3-D hexahedral (square) lattice

fill the lattice elements with various materials

create a universe 0 lattice

Problem - Square Array of Two layers of 6 $Pu(NO_3)_2$ Solution Cylinders

These chapters are followed by six appendices that provide the following information: Monte Carlo Techniques, Calculating Atom Densities, Specifications and Atom Densities of Selected Materials, Listing of Available Default Cross Sections, Geometry Plot and Tally MCPLOT Commands, and MCNP Surface Cards. The intent of the appendices was to make the primer as self-contained as possible with minimal requirements for outside references. Thus, some tables from the MCNP manual were included along with a brief discussion of how a Monte Carlo code works, and a tutorial on calculating atom densities.

The primer was completed in the summer of 1994 and first used in training in August 1994. The Transport Methods Group has distributed all but a very few of the four hundred twenty-five copies of the Primer that were initially printed. For reprints, we recommend contacting the Office of Scientific and Technical Information, P.O. Box 62, Oak Ridge, TN 37831 - phone (615) 576-8401.

TRAINING WITH THE PRIMER

In the past year, Group XTM has taught two classes with a specific focus on criticality calculations using the Primer as the text. The presentation of the material follows chronologically the exact order of the Primer. Lectures are only long enough to describe the material selected to discuss in that section and to describe the illustrative problem. Students working in pairs at a UNIX workstation then prepare an input file that models and plots the geometry, defines the materials, and provides the criticality control cards. MCNP is executed, using as input the file created. Finally, the output is discussed in detail with an emphasis on evaluating the quality of the calculation. The two main goals of the class are to teach users how to use MCNP correctly and efficiently, and to convince them that getting an answer is not the end of their job. They must check the output carefully to determine that the answer makes sense.

Experience with all our courses has convinced us that hands-on computer activity is essential for the student to "own" the material being discussed. It is one thing to sit and listen and entirely another to actually model the problem. Having expert guidance to help the student through parts that are not clear allows individual learning to occur in a timely manner. Students uniformly feel that they will be able to use the code knowledgeably when they return home after having actively participated in the learning process.

To keep the Primer to a manageable length, most chapters only list the final three-combined k_{eff} estimator value and estimated standard deviation. An advantage of the class is that the full output is discussed in significant detail. We strongly believe that MCNP should not be used as a black box. There are many features in the output that assist the user in determining the quality of the calculation. We emphasize that MCNP calculates a k_{eff} confidence interval. We impress upon the student that the criticality professional ultimately is responsible for certifying that the geometry assumptions, materials, and calculation are correct. To support this position, a Los Alamos criticality safety professional lectures in each class.

Although much of the information to do an analysis is provided in the primer, it is not a substitute for understanding the physics of a specific problem and the theory of neutron interactions. The MCNP code can only analyze the problem as specified; it will not necessarily identify inaccurate modeling of the geometry nor will it know when the wrong material has been specified. Without an understanding of the context of the problem, the quality of the solution, and a reasonable idea of what the result should be, a calculation of k_{eff} and its associated confidence interval with MCNP or any other code is meaningless.

The Primer is a document for a new user, as well as an excellent reference for an experienced user. Many times you see "For further information, refer to the the MCNP Manual." The class provides the opportunity to explain the more advanced information to the students. The grey bars in the Primer offer a thumbnail version of oftentimes complex topics. Even if the grey bar material is ignored, the Primer text flows seamlessly. One advantage of attending the class is that MCNP experts, building on the basics of the Primer, can increase the depth of understanding of all areas essential to the calculation.

One criticism of the examples used in the Primer, the same problems used in the class is that the dimensions and material descriptions are too complicated. For example, a sphere might have a radius of 6.38493 cm. or a material might have a Pu-239 atom fraction 3.7047e-2. These are real values as each example problem is drawn from a realistic critical system.[3] Therefore, while learning to use MCNP, students are also learning to interpret results produced from realistic calculations.

The k_{eff} -of-the-World Summary Problem

The last example problem used in the class is Elliot Whitesides' k_{eff}-of-the-world problem.[4] This problem consists of a 9x9x9 array of 4.7 cm radius plutonium spheres spaced 60 cm apart in a void. The assembly of 729 spheres is reflected externally by 30 cm of water. The k_{eff} of this system is about 0.92. The example problem, however, replaces the sphere at the center location with the critical Jezebel sphere, of 6.385 cm radius. The uniform-in-volume initial fission neutron source spatial distribution is deliberately chosen to differ significantly from the correct distribution, which is strongly peaked in the center. Because of this poor initial source distribution, it is much more difficult for the Monte Carlo power iteration method to adequately sample the critical Jezebel sphere and converge to the correct distribution. Reference 5 in these proceedings discusses this problem and the results in much more detail.

The class is asked to set up, plot, and run this problem with 1000 neutrons per generation, skipping 20 cycles and running 30 active cycles. This problem is easy to specify with the MCNP lattice capability and is a good geometry skills check after going through the more difficult MCNP Primer examples.

A complete MCNP output listing of this calculation is provided to each student. They are asked to analyze the output individually and to make a recommendation about the quality of the 99% k_{eff} confidence interval of 0.92 to 0.93. The correct result is 1.0 because Jezebel is in the problem. With only 50 cycles run and the poor initial source distribution, the critical Jezebel sphere is only beginning to be sampled adequately. Consequently, the MCNP analyses of the results are unable to detect the faulty confidence interval[5] because not enough k_{eff} cycles have been used. The difficulties in calculating a heterogeneous array with only about 1.4 neutrons per element based on 1000 neutrons per cycle and only 30 active cycles are stressed.

The class understands that the cycle-to-cycle power iteration method requires many cycles to adequately converge to the correct fission neutron spatial distribution from a poor initial distribution. The small number of neutrons per element per cycle is also strongly stressed as extremely undesirable for a heterogeneous system. The k_{eff} result is not yet acceptable and more cycles are required. Pictures of the fission source point locations as a function of cycle are shown to illustrate the source convergence process. Examples of these distributions are shown in reference 5.

The calculation is then continued to 120 total (100 active) cycles. MCNP now produced two WARNING messages: 1) the average k_{eff} is monotonically increasing for the last ten cycles; and 2) the first and second active half keff confidence intervals do not overlap at the 99% confidence level (0.92 to 0.94 and 0.96 to 0.98). The printed plots and other information provided by MCNP are studied. This calculation is clearly not acceptable because of the strong increasing trend in the average k_{eff}.

Finally, an output with 520 total cycles is discussed in detail. One WARNING message is produced: the first and second active half k_{eff} confidence intervals do not overlap at the 99% confidence level (0.95 to 0.96 and 0.99 to 1.00). The correct result can be found in the k_{eff}-by-cycles-skipped table by using the MCNP output analysis methods discussed during class.

The k_{eff} -of-the-world problem is an excellent criticality summary exer[illegible] because it checks understanding of geom[illegible], the Monte Carlo method, and MCNP output and WARNING message analyses. This problem forces the user to think about the Monte Carlo solution. The lessons learned from this problem are summarized with strong cautions that problem analysis by the user is ABSOLUTELY essential: no calculational result should be treated as a black box.

User Comments

Every student is given a critique sheet, and we provide a certificate of attendance in exchange for the critique on the last day. The course features found to be most useful include: 1) discussion of the continuous energy neutron physics, thermal treatments, and data libraries; 2) actually working out the exercises; 3) graphics for verifying geometry and viewing results; 4) detailed analysis of the output to assess the quality of the answer; 5) statistical concepts and the k_{eff} confidence interval[6]; and 6) the progressive nature of the Primer.

Suggested topics for more discussion are three areas barely touched on in the Primer: 1) standard tallies in a criticality calculation; 2) the general source capability, and 3) variance reduction methods. These three MCNP features can be very useful in criticality calculations and are taught in detail in other MCNP classes.

We encourage user feedback on the code and data libraries. The class provides an opportunity for Los Alamos MCNP code developers to interact with criticality users from around the world. Several improvements and additions to the code particularly for criticality were mentioned in the critiques and have been implemented in the latest version of MCNP. Examples include improved geometry plotting, k_{eff} graphics, WARNING messages, and installation procedures. Contacts with the students, via email, telephone, or at technical meetings, continue long after the class ends.

CONCLUSION

The criticality courses taught with the Primer as a text have been quite successful. The combination of having a text to follow that progresses from simple to complex, hearing more in-depth explanations of topics covered initially at a superficial level, and having the hands-on experience of participating in the learning experience allows students to feel confident when they return to their work place. Additionally, the Primer provides a uniformity from class to class for the instructors.

REFERENCES

1) Briesmeister, J. F., ed. "MCNP-A General Monte Carlo N-Particle Transport Code, Version 4A," Los Alamos National Laboratory Report LA-12625-M (November 1993).

2) Harmon, C. D., R. D. Busch, J. F. Briesmeister, and R. A. Forster, "Criticality Calculations with MCNP: A Primer," Los Alamos National Laboratory Report LA-12827-M, (August 1994).

3) Paxton H. C. and N. L. Pruvost, "Critical Dimensions of Systems Containing ^{235}U, ^{239}Pu, and ^{233}U," Los Alamos National Laboratory Report LA-10860-MS, 1986 Revision.

4) Whitesides, G. E., "A Difficulty in Computing the k-effective of the World," Trans. Am. Nucl. Soc., 14, 680 (1971).

5) Forster, R. A., Booth, T. E., Urbatsch, T. J., Van Riper, K. A., and Waters, L. S., "Visualization and Analyses of MCNP Criticality Results," ICNC '95 proceedings, Albuquerque, NM, 1995.

6) Urbatsch, T. J., Forster, R. A., Prael. R. E., and Beckman, R. J., "Understanding the Three-Combined k_{eff} Confidence Intervals in MCNP," ICNC '95 proceedings, Albuquerque, NM, 1995.