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TITLE: *MCNP CAPABILITIES FOR NUCLEAR WELL LOGGING CALCULATIONS*

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MCNP Capabilities For Nuclear Well Logging Calculations

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Abstract

The Los Alamos Radiation Transport Code System (LARTCS) consists of state-of-the-art Monte Carlo and discrete ordinates transport codes and data libraries. The general-purpose continuous-energy Monte Carlo code MCNP (Monte Carlo Neutron Photon), part of the LARTCS, provides a computational predictive capability for many applications of interest to the nuclear well logging community. The generalized three-dimensional geometry of MCNP is well suited for borehole-tool models. SABRINA, another component of the LARTCS, is a graphics code that can be used to interactively create a complex MCNP geometry. Users can define many source and tally characteristics with standard MCNP features. The time-dependent capability of the code is essential when modeling pulsed sources. Problems with neutrons, photons, and electrons as either single particle or coupled particles can be calculated with MCNP. The physics of neutron and photon transport and interactions is modeled in detail using the latest available cross-section data. A rich collection of variance reduction features can greatly increase the efficiency of a calculation. MCNP is written in FORTRAN 77 and has been run on a variety of computer systems from scientific workstations to supercomputers. The next production version of MCNP will include features such as continuous-energy electron transport and a multitasking option. Areas of ongoing research of interest to the well logging community include angle biasing, adaptive Monte Carlo, improved discrete ordinates capabilities, and discrete ordinates/Monte Carlo hybrid development. Los Alamos has requested approval by the Department of Energy to create a Radiation Transport Computational Facility under their User Facility Program to increase external interactions with industry, universities, and other government organizations.

1 Well Logging Calculations

The purpose of nuclear well logging is to determine the lithology and fluid characteristics of the materials surrounding the borehole by using neutron or photon radiation sources. The radiation interacts with the materials in and around the borehole. Sensitive detectors are used to measure the scattered radiation. Interpretations of these measurements are required to assess the properties of the surrounding material. The data interpretations usually are made based on benchmark measurements with the tool in a series of known borehole configurations, information from other logging tools, and detailed radiation transport calculations of the tool in the benchmark and downhole environments.

The purposes of the calculations are to predict and understand the measured results in as much detail as possible. Additional calculations can be used to provide calculated tool responses where measurement standards do not exist. Consequently, environmental corrections to the tool response resulting from changes in downhole conditions can be modeled using accurate radiation transport calculations. These calculations can provide detailed insight into the response of the tool, which is crucial to designing new or improved nuclear tools.

Nuclear well logging problems are difficult radiation transport calculations for several reasons. These problems are inherently three dimensional and are time dependent for pulsed radiation sources. The problems represent medium-to-deep radiation penetration and often require a coupled neutron-photon capability. Extremely accurate calculational results are needed to extract as much information as possible from the measurements. High accuracy requires an accurate representation of the source, a detailed geometric model, and the best and most extensive nuclear and atomic data that is available.

The Monte Carlo method addresses the complexities of time-dependent coupled-particle transport in complicated three-dimensional geometries using detailed continuous-energy data libraries. The MCNP code with its associated data libraries is well equipped to solve these kinds of difficult radiation transport problems.

2 Los Alamos Transport Codes

Los Alamos National Laboratory is a world leader in developing and applying the Monte Carlo and discrete ordinates methods to solving complex radiation transport problems. The result of this work has been the establishment of the

Los Alamos Radiation Transport Code System (LARTCS) that is comprised of six computer production codes used worldwide. The MCNP (Monte Carlo Neutron Photon) code[1] is used to calculate the time-dependent transport of radiation with Monte Carlo. The ONEDANT[2], TWODANT[3], and TWOHEX[4] codes use discrete ordinates with diffusion synthetic acceleration to calculate global steady-state radiation transport solutions to problems in one and two dimensions. The SABRINA[5] code is used to interactively setup three dimensional problems with a color graphics display of geometries and particle tracks. The final code in the system is the LAHET (Los Alamos High Energy Transport) code[6] that is used to transport neutral and charged particles with energies ranging from a few MeV to in excess of 10 GeV. Nuclear and atomic data libraries containing the best available data are also a crucial part of the LARTCS.

The remainder of this paper will discuss the MCNP code capabilities and data libraries with emphasis on nuclear well logging calculations.

3 MCNP History and Overview

The Monte Carlo method was developed at Los Alamos during the Manhattan Project in the early 1940s. During the 1950s, Monte Carlo machine language programs were written to solve transport problems. Cashwell and Everett[7,8] developed much of the mathematics of the Monte Carlo method that is still the basis for many of the MCNP algorithms. An updated Monte Carlo text by Carter and Cashwell[9] was written in 1975. MCS[10], the first Los Alamos general purpose Monte Carlo code, was written in 1963. The current MCNP code is based on its predecessors MCS, MCN[11], MCG[12], MCP[12], and MCNG. More than 350 person years have been invested into the research, development, programming, documentation, and data bases for MCNP.

MCNP is a general purpose Monte Carlo code for calculating the time-dependent continuous-energy transport of neutrons, photons, and electrons in either single particle or coupled particle mode in three-dimensional geometries. Both fixed source and k_{eff} criticality problems can be solved with MCNP. Data representations can be either fully or partially continuous or multigroup. MCNP is a production code in that a wide variety of transport problems are solved reliably and that a large number of input and execution error checks are made. The code is rich in variance reduction techniques that improve the efficiency of difficult calculations such as those in nuclear well logging. The documentation for MCNP is a 600-page manual[1] describing the Monte Carlo theory, geometry, physics, cross sections, variance reduction techniques, tallies, errors, input, and output. Many examples assist the user to setup problems, to make efficient calculations, and to interpret the results.

4 MCNP Physics Data

An important part of MCNP is the extensive continuous-energy and multigroup data libraries available with the code. Accurate calculations require accurate data.

The neutron data libraries are derived from three sources and cover the energy range from 10^{-11} to 20 MeV. Ninety evaluations are based on the most current information from ENDF/B-V (Evaluated Nuclear Data File) data. Ninety-two evaluations are available from ENDL-85 (Evaluated Nuclear Data Livermore) data. For data needs that could not be met with either of the above libraries, the Los Alamos Applied Nuclear Science Group T-2 has provided 17 special evaluations. All data are represented in the full detail required to faithfully reproduce the evaluators' intentions. For some data sets, there are well over 10000 energies at which cross sections are tabulated. In addition, there are typically dozens of energy-angle tables at various incident neutron energies for each neutron-producing reaction.

Low energy neutrons are treated in two different ways. The first and most detailed and accurate treatment is the $S(\alpha,\beta)$ data that includes molecular and crystalline binding effects at specific temperatures in selected materials (presently, H_2O,D_2O,Be,BeO,ZrH_2, polyethylene, graphite, and benzene). The second treatment is the free gas model where the nuclei are assumed to be a gas having an isotropic Maxwellian distribution of velocities that is dependent on the temperature of the material.

In addition to the neutron transport data discussed above, a neutron dosimetry library is available for selected isotopes. This library contains data for specific neutron reactions that are used to calculate responses such as reaction rates and particle production rates when folded with calculated neutron fluxes.

For coupled problems, detailed neutron-induced photon data are included for all evaluations for which the data exist. All of the energy-dependent and energy-independent photon lines and continuum distributions are included in these data to provide the capability to calculate detailed photon spectra. These characteristic photon lines and their intensities are important for calculating the detailed (n,γ) response for nuclear well logging tools.

The MCNP photon interaction library contains data based on the ENDF/B-V evaluations plus Storm and Israel evaluations for a few high atomic number isotopes. The energy range for photon transport in MCNP is between 10^{-3} and 100 MeV. This library contains data for pair production, incoherent and coherent scattering, and photoelectric absorption followed by the emission of one or two fluorescent photons above 1 KeV.

Given appropriate cross-section data, forward and adjoint transport calculations for any type and combination of neutral and charged-particles can be done with a new hybrid continuous-energy/multigroup Boltzmann-Fokker-Planck treatment[13]. At the present time, cross-section data is available only for coupled electron photon calco lations. These data are generated by a special version of the CEPXS code[14]. This new capability is available for production calculations, but is not yet mature. Further experience is needed to fully characterize and optimize the algorithm. (A mature capability now exists for 1-D discrete-ordinates coupled electron-photon transport calculations using CEPXS together with a new version of ONEDANT called ONEDANT-LD[14].)

5 MCNP Material Specifications

Materials for MCNP problems are defined by selecting combinations of isotopes and elements from the data libraries. Either atomic fractions or weight fractions are entered to specify the composition of a material. Default neutron cross sections are available or specific evaluations at appropriate temperatures are selected. $S(\alpha,\beta)$ low energy neutron data can be associated with any material. Cell-dependent and time-dependent temperatures can be input for appropriate low energy neutron treatment with the free gas model.

6 MCNP Cells and Surfaces

Cells are the basic geometric unit in MCNP. They locate materials and are used for volume tallies and variance reduction parameter specification. Surfaces are used to create cells in Cartesian coordinates using the mathematical sense of space on either side of the surface. Surface tallies are made on surfaces. Cells are constructed using the Boolean intersection, union, and complement operators. Parentheses control the order of execution of the three operators. Specification of cells using body geometry is available with SABRINA. A general repeated structures capability is available to reduce geometry setup time when portions of the geometry appear more than once.

MCNP allows easy specification of cells with skewed surfaces. Such a cell can be defined in a convenient auxiliary Cartesian coordinate system. The relation between the auxiliary system and the primary system then is supplied to the code by the user.

MCNP surfaces are defined by all first- and second-order equations and certain fourth-order equations (elliptical tori). There are 26 surfaces available that are specified by equation coefficients. Certain surfaces can be specified by points as well. When symmetry exists in the geometry, reflecting surfaces simplify the problem setup and improve the efficiency of the calculation.

MCNP provides graphics to view the geometry and detect errors. Any arbitrary 2-D geometrical slice can be plotted. Dashed lines indicate geometry errors. Any of 18 problem parameters can be displayed by cell on these plots. Length scales can be included on the plots if desired.

The SABRINA code produces either 3-D color-shaded or 3-D line plots of a geometry. This graphics capability plus the interactive features allow SABRINA to reduce significantly the effort required to construct a complicated MCNP model. The test option in SABRINA is useful for finding errors in the model. The code can show actual Monte Carlo particle tracks superimposed on the geometry.

7 MCNP Sources

MCNP has a highly generalized fixed source capability to specify a radiation source at a point, on a surface, in a cell, or any combination of the three. Source variables can be defined as a value, as an independent distribution, or as a distribution dependent on another source variable. All input source parameters can be biased in various ways by the user. A subroutine SOURCE exists so the user can write his own coding, but this is seldom needed.

When a problem can be separated into two or more parts, a particle surface source option is available. For this source, MCNP writes a file containing information about particles crossing one or more surfaces. This file can be used in subsequent calculations to study various geometries on the other side of the surfaces without having to rerun the initial problem. This feature can be useful for designing detectors and their spacing in well logging tools.

8 MCNP Variance Reduction

Analog Monte Carlo calculations, where the particles' random walks directly follow the physical processes, are usually effective only for problems where substantial numbers of particles are in the tally regions. For more difficult problems, such as those that occur in nuclear well logging, variance reduction techniques using nonanalog schemes must be used. These techniques combine particle weight control and sampling from biased probability density functions with particle weight corrections to increase problem efficiency, sometimes up to many orders of magnitude.

MCNP has many sophisticated variance reduction techniques that have been developed for and thoroughly tested on a wide variety of Los Alamos problems. Presently, there are the following 15 techniques in MCNP: importance splitting and Russian roulette, weight cutoff with Russian roulette, energy splitting with Russian roulette, time cutoff, energy cutoff, implicit capture, exponential transform, forced collisions, correlated sampling, source biasing, various forms of the point detector tally, DXTRAN, neutron-induced photon source weight control and line selection, and weight windows. Many of these techniques are used together routinely to produce more efficient Monte Carlo solutions to nuclear well logging problems. The application of MCNP variance reduction techniques to a sample problem is discussed in reference 15.

One of the newest techniques in MCNP is the weight window that keeps the particle weights within defined limits as a function of energy and cell. Weight windows must be used with care and with some physical insight into the problem. MCNP has a weight window generator[16] to determine appropriate window parameters by running the equivalent of an adjoint calculation in the forward mode. The weight window generator and the weight window have been successfully applied to a variety of problems, including well logging. More information on the weight window and all of the MCNP variance reduction techniques is available in the MCNP manual.

9 MCNP Tallies

MCNP can tally by particle type the radiation particle quantities of flux, current, and heating. The only limit to the number of tallies in a problem is computer memory. All tallies can be made as a user-specified function of space, energy, and time. Fluxes can be tallied in a volume or in portions of a volume, on a surface or on portions of a surface, or at a point or at a point on a ring. Particle current tallies are made on surfaces or on portions of surfaces with the cosine of the angle of crossing relative to the surface normal as another tally variable. Heating (energy deposition) tallies by cell or portions of cells are also available.

The quantities required for the calculation of the estimated relative error of each tally result are calculated at the end of each history. A figure of merit, defined to be the inverse of the relative error squared times the computer time, is provided for each tally by history number. This quantity is useful for determining if a tally is statistically well behaved and for optimizing the overall efficiency of a calculation.

MCNP contains many features to convert fluxes to reaction rates or to modify fluxes by response functions. There are user-specified bin multipliers and energy functions available. It is easy to multiply fluxes by sums and products of any the reaction cross sections of a material to produce desired reaction rates. Other useful features in the code for well logging problems are flagging tallies by the cells or surfaces that the particles cross, tallying by the collision number of the particle, and providing a time convolution for a much more efficient calculation for a square-wave pulsed source. If the desired tally is not available, the user can define any modified tally by providing coding for subroutine TALLYX that is called just before a tally is posted.

MCNP automatically provides summary information about the particles' random walks and collisions in every cell in the problem. A ledger table of track, weight, and energy gains and losses by physical and variance reduction categories is also printed. Users should understand the information in these tables to understand the particle transport in the problem.

All tally results can be displayed by MCNP in 2-D X-Y, 2-D contour, or 3-D surface plots. The results can be represented as a histogram, as a piece-wise-linear curve or spline curve between points, or in bar graph form. Plotting the error bars is optional. Multiple plots can be made on the same axes, tally results can be scaled, and data from other sources can be plotted.

10 MCNP Software

MCNP is written in ANSI-standard FORTRAN 77 and uses the Los Alamos Common Graphics System (CGS), GRAFLIB, PLOT10, DISSPLA, or DI3000 graphics. There are approximately 28500 lines of unexpanded source code in about 300 subroutines that are logically structured and quite readable. Virtually all storage arrays are dynamically allocated, keeping each problem as small as possible on the computer. The MCNP software is designed to be modified by users. All variables that appear in COMMON are defined in the MCNP manual.

MCNP is maintained as a single source code. To achieve portability, a preprocessor for the source code is required such as UPDATE, HISTORIAN, or MCNP's own portable preprocessor. The preprocessor generates a source deck with the appropriate COMMON decks and conditional compilation directives for the specified computer system. The data files and graphics are also portable. To date, MCNP has been compiled, loaded, and run on at least the following machines: Cray (CTSS, COS, and UNICOS), CDC (NOS), IBM, VAX, PRIME, SUN, APOLLO, ENCORE, and RIDGE.

MCNP is distributed for Los Alamos by the Radiation Shielding Information Center (RSIC) in Oak Ridge, Tennessee. They receive about 50 requests per year for MCNP. RSIC provides a copy of the code and documentation for each request and answers questions concerning installing the code on different computers. Requests for MCNP should be directed to RSIC.

11 MCNP Usage & Applications

Version-to-version quality assurance is verified by running and checking a variety of test problems that, as a set, exercise the features of the code. MCNP and its data libraries are benchmarked by extensive use on real transport problems with measured results at Los Alamos and many other institutions. MCNP is run about 300 Cray hours per month at Los Alamos alone. About 100 different Los Alamos users apply MCNP to a variety of problems including criticality analysis, nuclear safeguards, nuclear reactor and shielding designs, magnetic fusion energy neutronics, nuclear instrument design and analysis, physics experiments, radiological doses, and nuclear well logging. There are many reports and publications in journals and professional society transactions documenting the application of MCNP to these problems.

12 Version 4 of MCNP

Version 4 of MCNP has been under development for the last two years and will provide several new capabilities. This version has been restructured internally so that other kinds of particle physics can be added to the code with a minimum of effort. MCNP will stand for Monte Carlo N Particle, to emphasize the expanded scope of the code. As a first step in this direction, electrons have been added as a third particle type. A continuous-energy electron transport package and associated data based on the Integrated Tiger Series[17] developed at Sandia National Laboratory has been incorporated into MCNP. A thick target Bremsstrahlung electron-induced photon production model using these data has also been incorporated into Version 4 to include much of the electron physics for photon generation at a fraction of the cost of the fully continuous-energy electron treatment.

Another important addition to MCNP is a shared memory multitasking capability. The clock turnaround for multitasked problems is reduced by approximately the number of processors used in the calculation. The code has been successfully multitasked on the Los Alamos Crays and the Apollo scientific workstation. Multitasking for other systems will require special modifications to MCNP because of the highly nonportable aspects of parallel processing.

There are many other improvements to the code. One of special interest for nuclear well logging calculations is the addition of a pulse-height detector tally. This tally records the energy deposited in a cell by each source particle and its secondary particles. This new type of tally is different from all other tallies in MCNP because the microscopic events must be modeled as realistically as possible. Except for special cases, source biasing is the only variance reduction technique allowed with the pulse-height tally.

Additional testing is required on Version 4 before it goes into production status at Los Alamos and then is released to RSIC. A tentative time frame for this release is Spring 1990.

13 Future Directions

The long term vision for the LARTCS is further integration and expanded capabilities for the components of this system. Los Alamos will continue work in research and development of the Monte Carlo and discrete ordinates methods toward solving ever more challenging transport problems and problems in other areas where the methods apply. Because of its unique transport and data expertise, Los Alamos has requested that a Radiation Transport Computational Facility (RTCF) be formed as an "other user resource" under the Department of Energy User Facility Program. The goal of the RTCF is to increase external interactions for research, code and data development, and applications.

The future directions in all of the technical areas depend on future funding sources. Work is proceeding on improved angle biasing methods and phase-space importances that should improve the efficiency of MCNP for all transport problems, including nuclear well logging. Work needs to be done to establish variance reduction techniques that can be used with the new pulse-height tally. The present formulations are correct for tallies that are sums of individual tracks. The variance reduction techniques are usually not correct for pulse-height detector tallies because the collective effects of several tracks contributing to the tally are not included.

One extremely promising research area currently being pursued at a low level is adaptive Monte Carlo, where the computer learns the most important paths through particle phase space for a particular problem. At Los Alamos, adaptive Monte Carlo was first applied to a discrete-state transport problem and exponential (versus square root) convergence was observed[18]. An adaptive technique presently being investigated for continuous transport problems is called "intelligent random numbers," where biasing takes place in random number space[19,20]. The technique has been partially tried in MCNP to automatically learn to divide phase space into importance regions[21]. Much work remains to be done, but the payoffs could be enormous in terms of the computer savings and the more difficult problems that could be solved.

In the discrete ordinates area, a small effort is being expended on three-dimensional transport using faster algorithms with capabilities such as diffusion synthetic acceleration. Additional areas of importance to nuclear well logging that deserve attention are generalized geometry, time dependence, efficient multitasking algorithms, and appropriate links between discrete ordinates and Monte Carlo. Once available, these improved discrete ordinates capabilities could contribute heavily to the understanding of nuclear well logging tool responses.

Our data bases will continue to be improved as much as possible to provide the latest evaluations. In the near future, ENDF/B-VI will become available and has, among other things, improved representations of particle energy-angle correlations. To intergrate the new evaluations into MCNP will require considerable effort because of the new data structures.

14 Summary

The codes in the Los Alamos Radiation Transport Code System are user-oriented production codes that are run extensively at Los Alamos and elsewhere to solve many types of transport problems. The associated nuclear and atomic data bases are the best available and contain all of the information in each evaluation in as much detail as possible. MCNP and its data libraries are well suited to produce accurate transport solutions to the difficult class of problems in nuclear well logging. A small amount of work is under way to develop and implement new techniques in both our discrete ordinates and Monte Carlo codes that will improve our capability to solve transport problems in general and nuclear well logging in particular. It is hoped that, with the approval of the Radiation Transport Computational Facility by the Department of Energy, Los Alamos can have increased interactions of mutual interest with other organizations in areas of radiation transport.

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