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THE STATUS OF MONTE CARLO AT LOS ALAMOS

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ABSTRACT

At Los Alamos the early work of Fermi, von Neumann, and Ulam has been developed and supplemented by many followers, notably Cashwell and Everett, and the main product today is the continuous-energy, general-purpose, generalized-geometry, time-dependent, coupled neutron-photon transport code called MCNP. The Los Alamos Monte Carlo research and development effort is concentrated in Group X-6.

MCNP treats an arbitrary three-dimensional configuration of arbitrary materials in geometric cells bounded by first- and second-degree surfaces and some fourth-degree surfaces (elliptical tori). MCNP has its own cross-section libraries plus it allows two thermal neutron models: the free-gas and $S(\alpha,\beta)$ treatments. There is a wide variety of standard sources plus a very easy-to-use and extensive tally structure. MCNP is quite rich in variance-reduction schemes, including three different techniques for estimating flux at a point. Other features include being able to calculate eigenvalues for both sub- and super-critical systems, an elaborate plotter for checking geometry setups, calculation of cell volumes and surface areas, and good documentation.

Monte Carlo has evolved into perhaps the main method for radiation transport calculations at Los Alamos. MCNP is used in every technical division at the Laboratory by over 130 users about 600 times a month accounting for nearly 200 hours of CDC-7600 time. However, MCNP is just the parent code. In addition to MCNP, major variants supported by Group X-6 include a multigroup forward and adjoint code, a code allowing geometrical perturbations, and a code that allows cell boundaries to change as a function of time. In addition, Group X-6 is involved in electron and high-energy nucleon/meson transport by Monte Carlo.

INTRODUCTION

We are happy to report that Monte Carlo is alive and well at Los Alamos. Our main code, MCNP,[1] is used by about 130 users in virtually every technical division at the Laboratory over 600 times a month, accounting for nearly 200 hours of CDC-7600 computer time. Monte Carlo, and in particular MCNP, is possibly the main method for radiation transport calculations at Los Alamos today. MCNP is also actively supported by Group X-6 on the Magnetic Fusion Energy computer network where it is used by a number of people throughout the country. Although Monte Carlo has widespread use at Los Alamos, the main research, code development and maintenance, user support, documentation, and nonroutine applications are concentrated in Group X-6 in the Theoretical Applications Division (X-Division). The purpose of this paper is to tell you a little about X-6 and its codes, with emphasis on MCNP.

GROUP X-6

Group X-6, presently consisting of 22 members, has as its title "Monte Carlo, Applications, and Transport Data." From this title, it is clear we have three areas of concern: (1) Monte Carlo methods and code development, (2) applications requiring particle transport by Monte Carlo, and (3) cross-section data. A strength of the group lies in the interaction of these three areas and their support of one another. To a very large extent, all the people in X-6 are conversant in each of these areas and appreciate the requirements and problems of each. The magnitude of the Monte Carlo expertise that resides in X-6 is likely unrivaled.

Activities in each of these areas will be discussed, but to help clarify the role of Group X-6 relative to some other activities at Los Alamos that you may be familiar with, the role of two groups from the Theoretical Division will be briefly mentioned. Group T-1, headed by D. J. Dudziak, is where the Laboratory's S_n expertise is concentrated. They are responsible for codes like ONETRAN[2] and TRIDENT.[3] Like X-6 they also are involved in applications but specialize in S_n and occasionally use the X-6 Monte Carlo codes as we in X-6 occasionally use their S_n codes. Basically though, we in X-6 solve transport problems randomly and T-1 solves transport problems discretely. Group T-2, headed by P. G. Young, is the Laboratory's nuclear data group. Among other activities, T-2 evaluates cross sections and processes data sets with their codes such as NJOY;[4] X-6 does not evaluate cross sections but extensively tests them and then makes them available in proper form for direct use by many of the major transport codes at LASL.

Monte Carlo Methods and Code Development

X-6 responds to requests from throughout the Laboratory for new methods and techniques to help solve individual problems. The requests are frequently very specific and limited in scope (such as how to sample from some exotic distribution), but the requests may lead to a new feature that becomes a permanent part of our codes. Furthermore, X-6 originates many new methods and code improvements based on its knowledge of Monte Carlo and applications.

Some of the recent accomplishments include an S(α,β) thermal treatment, a more general analytical volume and surface-area calculator,[5] a very general tally structure, a once-more-collided point detector routine with a bounded variance, the addition of the union and complement operators for geometry specification, new standard sources with improved directional biasing into a fixed cone or in a continuous manner by means of an exponential function, a way to deterministically transport particles during their random walk (DXTRAN), many more user-oriented features and safeguards, plus a long list of miscellaneous items. A major accomplishment has been in the area of code documentation with the publishing of the 411-page MCNP manual[1] that contains over a hundred pages each of theory, cookbook examples, and details of the coding.

In the area of Monte Carlo theory, the theory of errors is a significant topic in X-6,[6-9] and a major work on relativistic effects has just been published.[10]

A new area of code development and physics for X-6 is the transport of high-energy (GeV range) protons, pions, mesons and the complete cascade of secondary particles down to the thermal-energy range. Applications will include energy deposition calculations in tissue in conjunction with the Los Alamos Meson Physics Facility research in cancer treatment plus shielding and materials damage studies. Our work is based on a modification to the HETC[11] code with an interface to MCNP.

In addition to the parent code MCNP, other X-6 codes include MCMG[12] which is a multigroup version of MCNP that also has an adjoint capability, MCNPPER that allows geometrical perturbations for calculating derivative information, MCNE which is a coupled electron-photon code that addresses the complete electron-photon cascade in the energy range from 20 MeV to 100 keV, a code that allows geometrical boundaries to change as a function of time, and numerous special versions of MCNP with which we evaluate new techniques and solve specialized problems.

About 40% of our effort is spent in this area.

Applications

X-6 serves two roles in the area of applications: (1) we work closely with MCNP users to help them with their applications, and (2) we do many applications ourselves that require our expertise and experience. Both these roles are valuable because they give us feedback on the use of MCNP and how best to improve it, and they broaden our own experience with a variety of applications.

Many applications are related to data verification and will be mentioned in that context.

An ongoing responsibility that we have for the Laboratory is calculating the biological dose from the intrinsic radiation (from the various natural decay modes of plutonium and uranium isotopes) emitted from the nuclear material used in nuclear weapons. This is of concern when military personnel are required to be in the proximity of the weapons for extended periods of time as is the case on a submarine. We also perform many calculations related to the vulnerability and effects of nuclear weapons.

X-6 has done extensive neutronics calculations for magnetic fusion reactor designs such as the Elmo Bumpy Torus (EBT),[13] Linus,[14] Reversed Field Pinch Reactor (RFPR)[15] and Fast-Liner Reactor[16] concepts. Furthermore, studies were made on Tokamak designs to evaluate the effect of geometrical simplifications in calculations.[17] Figure 1 is a Tokamak reactor geometry set up for MCNP; the surfaces marked by asterisks are tori. We would like to increase our role in the magnetic fusion area.

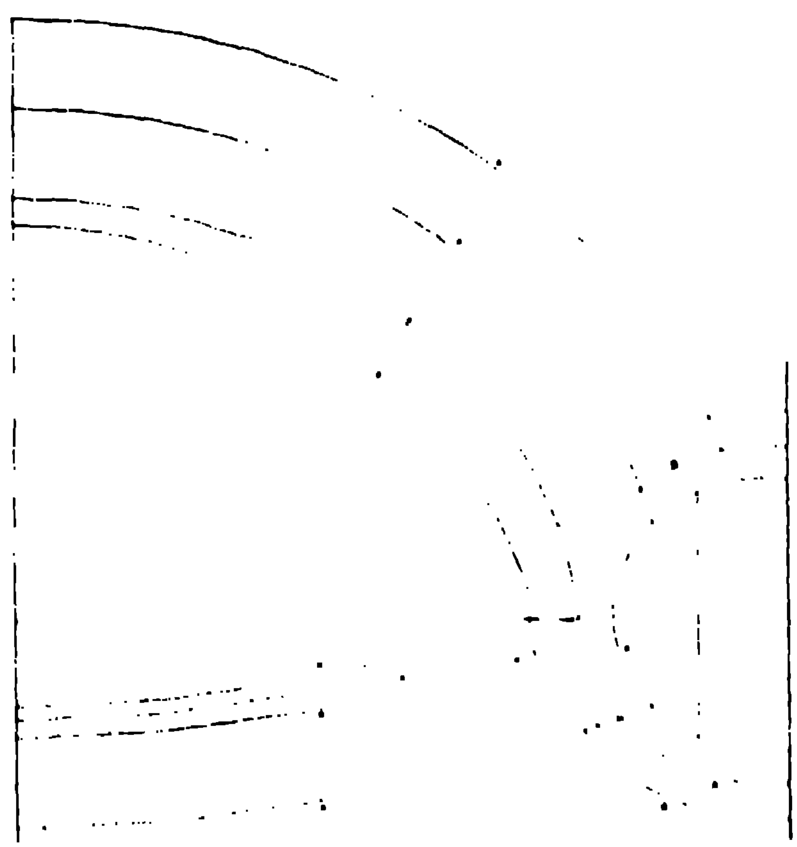

Figure 1. Tokamak Geometry.

The shielding designs for new facilities to be built at Los Alamos are frequently done by X-6. Recent examples include shielding from bremsstrahlung for a new electron accelerator to be built by the Physics Division and for the Antares Laser Fusion facility being built by the Laser Division. The Monte Carlo bulk-shielding calculations were done for Antares during the early design of the facility.[18] The basic building has been constructed, and we are now doing a radiation mapping inside the Target Building to ascertain material and instrumentation damage plus activation analysis of the target-chamber components. Figure 2 is the MCNP representation of the Antares target-insertion mechanism.

An activation analysis code, using the LASL GAMMON library,[19] is coupled with MCNP and calculates gas production (H,D,T, and He), material activation, and photon sources. The photon sources can be used in MCNP to calculate dose rates at points of interest.

Figure 2. Antares Target-Insertion Mechanism.

Many interesting calculations have been done for the Health Division that involve instrument design[20,21] and radiation safety. One project involved the design of the gloveboxes at the new Plutonium Facility at Los Alamos, and another project just completed was a criticality study for the Slagging Pyrolysis Incinerator Facility (SPI) to be built at Idaho Falls.[22]

A recent series of calculations was completed as part of the review of the design of the Fusion Material Irradiation Test Facility (FMIT) to be built at Hanford.

X-6 works closely with the Nuclear Safeguards (assay and accountability) groups at Los Alamos in the designing of instrumentation, helping to understand the physics and Monte Carlo simulation of their experiments, and providing special versions of MCNP to account for delayed neutrons and to simulate coincidence counters.[23] Calculations in this area are invaluable to optimize an instrument design and to understand or extrapolate a calibration curve in the assay of unknowns.

About 35% of X-6's effort is spent in the area of applications.

Transport Data

X-6 is responsible for the X-Division nuclear cross sections and does partial processing of cross-section data provided by Group T-2. This includes continuous-energy, multigroup, and radiochemistry data used not only in the X-6 Monte Carlo codes but also in other transport codes used in X-Division and throughout the Laboratory.

The major effort in this third area of X-6 work is the testing of cross-section data.[24] The data are verified by two methods: (1) differential testing involving spectra, and (2) integral testing involving critical mass calculations of Los Alamos assemblies like Godiva and Jezebel. As part of this cross-section work, X-6 has been calculating and analyzing the latest experiment designed to measure the neutron spectrum and tritium production, and to check specific cross sections at various locations in a system consisting of a 93.5% enriched uranium sphere surrounded by ^{6}LiD. The Livermore pulsed-sphere experiments are also calculated for integral testing of cross-section data.

Extensive thermal benchmark calculations have recently been completed to test the integrity of MCNP, its thermal treatments, and its data.[25] MCNP calculations are now making significant contributions to the thermal data-testing program.

We have recently completed the monumental task of thinning, testing, and assembling in suitable form the ENDF/B-V and Livermore ENDL79 data. These data are now being used at Los Alamos.[26-28]

This final area accounts for about 25% of the group's effort. We find having this cross-section effort an integral part of X-6 to be a very valuable arrangement. It gives those of us doing applications a greater appreciation and awareness of the data. Furthermore, great resources can be immediately brought to bear on questions of transport data - as illustrated in the following paper on deep-penetration calculations by Thompson, Deutsch, and Booth.

MCNP

As mentioned earlier, Group X-6 is the author of MCNP, and MCNP is the backbone and main product of X-6.

MCNP is a very mature and reliable Monte Carlo code. It represents over two hundred man-years of effort and is the culmination of the original Monte Carlo work at Los Alamos by Fermi, von Neumann, and Ulam. Cashwell and Everett, over a period of almost thirty years, have contributed most to the development of MCNP. Thew first book on MCNP was written by Cashwell and Everett.[29]

MCNP is a general-purpose, continuous-energy, generalized-geometry, time-dependent, coupled neutron-photon Monte Carlo transport code. It may be used in any of three modes: (1) neutron transport only, (2) combined neutron-photon transport, or (3) photon transport only. The capability to calculate eigenvalues for critical systems is also a standard feature of MCNP.

The following few sections will point out the main features of MCNP but will not go into detail. The MCNP manual, in addition to explaining how to use the code, contains the details of the physics, mathematics, and nuclear data aspects of MCNP. Another short publication,[30] which is just a reprint of the first part of the manual, summarizes the code. Finally, Carter and Cashwell's book[31] is not only a good general reference on radiation transport by Monte Carlo, but it is based upon MCNP in many aspects.

For most applications of MCNP, the user has to supply no more than an input file describing a problem. All of the input to MCNP is in free format. There is a variety of standard sources to choose from, and the tally structure is very general and elaborate. There is no need for a user to compile cross-section libraries for problems; X-6 maintains and provides all the data needed by MCNP.

Nuclear Data and Reactions

MCNP is a continuous-energy Monte Carlo code that makes no gross approximations regarding data. Linear interpolation is used between energy points with a few hundred to several thousand points typically required to reproduce the original data within a specified tolerance (in fact, usually within 0.1 to 0.5%). The only significant difference between the MCNP data libraries and the ENDF/B library (from which it is derived with the NJOY processing code) is that resonance data are represented in MCNP as linearly interpolated pointwise data that are Doppler broadened to a specific temperature. All reactions given in a particular neutron cross-section evaluation are accounted for in the energy range from 20 MeV to 10^{-5} eV. Users can choose from data with prompt or total fission ν's as well as having the option to use a set of discrete-reaction cross sections in which the reaction cross sections have been collapsed into 240 energy groups to save computer memory. Users have the choice of data from the ENDF/B, British AWRE, Livermore ENDL, or special LASL libraries.

There are two thermal treatments in MCNP. One is the free-gas model in which, for elastic collisions, light atoms (Z = 1 through 8) are assumed to be in a Maxwellian distribution with some thermal temperature that may be a function of time. Secondly, the $S(\alpha,\beta)$ scattering model is available which accounts for chemical binding and crystalline effects at very low energies. Typically, when going down to room temperature, the free-gas model is used from around 10 eV to 4 eV, and then the $S(\alpha,\beta)$ model is used below that.

Photon interactions are accounted for in the range of 100 MeV to 1 keV. MCNP accounts for both incoherent and coherent scattering, fluorescent emission following photoelectric absorption, and pair production.

Geometry

The geometry of MCNP treats a general three-dimensional configuration of arbitrarily-defined materials in geometric cells bounded by first- and second-degree surfaces and some special fourth-degree surfaces (elliptical tori). The cells are defined by the intersections, unions, and complements of regions bounded by the surfaces.

Surfaces are easily defined by supplying coefficients to the analytic surface equations or by indicating known points located on the surfaces. For example, the surface y - D = 0 is represented in MCNP by the mnemonic PY with the single entry D. Therefore, a plane normal to the y-axis at y = 4 is defined by the simple input line of

PY 4

MCNP has 26 such mnemonics available.

Figure 3 is a geometry set up to test the analytical volume calculator in MCNP (the volume was calculated analytically and also stochastically by using a track-length estimator). This geometry of a fancy fish with a weird sun is actually only three cells in the MCNP problem: (1) the disjoint regions of the fish plus the sun (which appears as four regions), (2) everything else inside the sphere, and (3) everything outside the sphere. The geometry was specified by portions of twenty-three surfaces consisting of six tori, two hyperboloids, two ellipsoids, seven cones, one cylinder, two spheres, and three planes.

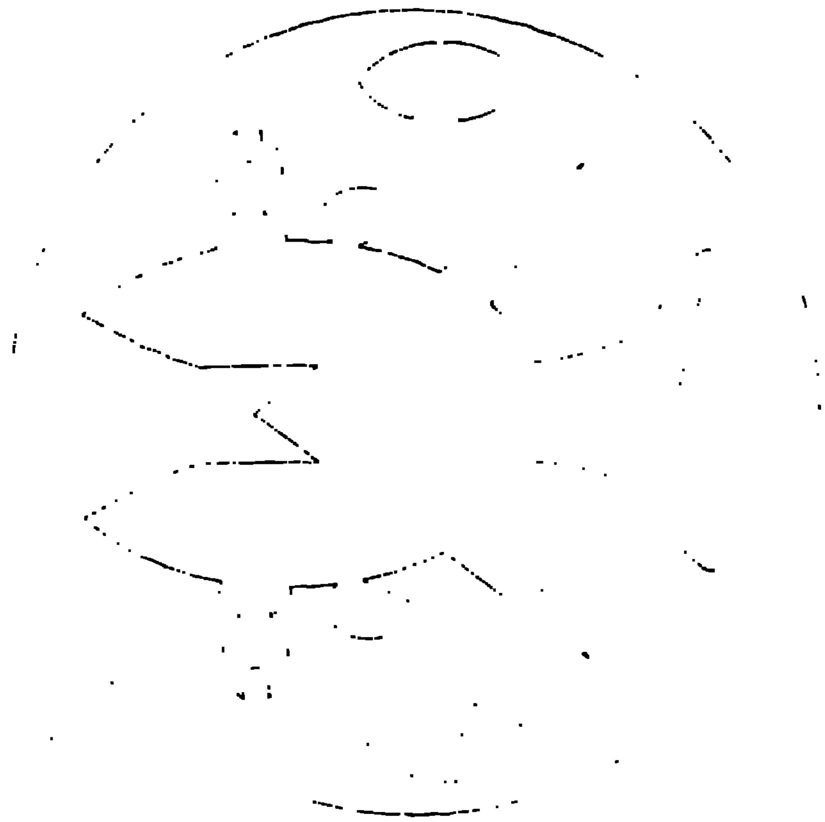

Figure 3. Example of MCNP Geometry.

Figure 4 is another example of MCNP geometry. This geometry consists of two cells and fifteen surfaces. The numbers in the figure refer to surface numbers: surface 1 is a cylinder; 3 is a cone; 12 and 13 are planes; 6, 7, 14 and 15 are ellipsoids; and 2, 5, 9, 10, and 11 are planes of two sheets.

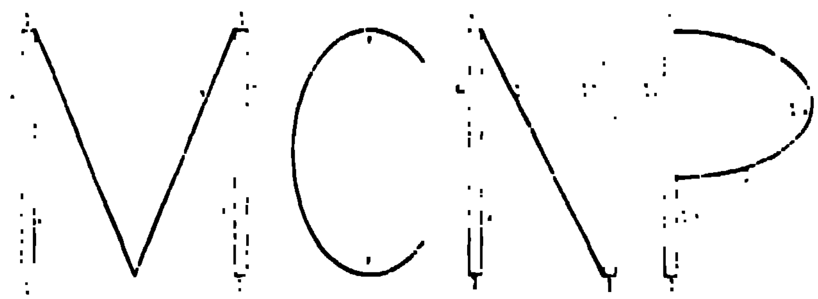

Figure 4. Example of MCNP Geometry.

More details about the MCNP geometry are given in the following paper by Godfrey. The significant additions of the union and complement operators to our geometry vocabulary are products of Godfrey's work. Cells that are now routinely specified with the union operator that are illegitimate when using intersections only are now in fact called "Godfrey cells" by us.

Variance Reduction

This one area alone makes MCNP a superb Monte Carlo code; MCNP is rich in variance-reduction techniques. The following two papers by Cashwell and Schrandt and by Thompson, Deutsch, and Booth will illustrate some of these techniques. More details are available in Refs. 1 and 31.

In addition to obvious ways to save computer time like using energy and time cutoffs, MCNP offers geometry splitting with Russian roulette, analog capture or survival biasing with weight cutoff and Russian roulette, correlated sampling, the exponential transformation, energy splitting, forced collisions, flux estimates at points by three methods (next-event estimator, ring detector, and once-more-collided estimator), track-length estimators, source biasing in direction and energy, and a combination random walk/deterministic scheme called DXTRAN. Furthermore, a Russian roulette game can be played with detector or DXTRAN contributions as a function of mean free path that can save substantial computer time.

X-6 is always evaluating new variance-reduction techniques and improving existing ones. Examples are (1) angle biasing which we look at from time to time but to date have not found a scheme that has anything substantial to offer over other methods already in MCNP, and (2) a weight window that looks quite promising (see paper by Thompson, Deutsch, and Booth). Furthermore, we are looking at generalized phase-space splitting.

Tallies

An important part of the MCNP output that the user has little control over (except for all of it or a fixed subset of it) is summary and diagnostic information. This information is valuable for determining the characteristics of a problem and the effect of variance-reduction techniques. Examples are (1) a complete breakdown of all energy and weight creation and loss mechanisms averaged over the entire problem and also individually by cell, (2) the number of tracks entering a cell and the track population in a cell, (3) the average energy, weight, number of collisions, and mean free path in a cell, (4) the volume, mass, and surface area of a cell, and (5) the activity (i.e., collisions, collisions times weight, and weight lost to capture) of each nuclide in each cell.

In addition to this summary information, MCNP has an elaborate and easy-to-use tally structure that allows the user to tally almost anything conceivable. Choices include, as a function of energy and time,

(1) current as a function of direction across a surface, (2) flux across a surface, (3) flux at a point, (4) average flux in a cell, and (5) energy deposition (or heating) in a cell by neutrons, photons, and products of neutron reactions. Surfaces or cells may be subdivided into segments for tallying purposes. In addition, particles may be flagged when they cross specified surfaces or enter designated cells, and the contributions of these flagged particles to the tallies are listed separately. The user has available a special subroutine by which the standard tallies can be modified in almost any desired way.

Reactions such as fission, absorption, tritium production, or any product of the flux times the approximately one hundred standard ENDF/B reactions plus several nonstandard ones may be tallied very simply.

Printed out with each tally is also its estimated relative error corresponding to one standard deviation of the mean.

Other Features

MCNP has the capability to calculate eigenvalues for critical systems. Three estimators (in various combinations) are used to calculate k_{eff}: absorption, collision, and track-length estimators.

For debugging input and geometries, MCNP makes extensive and elaborate checks for consistency. A plotting capability is in MCNP that provides an arbitrary cross-sectional view of the input geometry on several output devices (all figures in this paper plus slides used in the oral presentation were generated by the plotter). If a track gets lost during its transport, diagnostics are automatically printed for that track which include an event log. The event log is a print of the complete life of the track from event to event (birth, collisions, surface crossing, etc.).

A feature is available to allow the user to translate and/or rotate surfaces from one coordinate system to another. For example, it is a nontrivial task to determine the coefficients for the general quadratic equation needed to define an ellipse with its origin off somewhere in space and its axes at some skewed angle. However, an ellipse can be easily defined centered about the coordinate-system origin with axes parallel to the coordinate axes. It is then an easy procedure to move the simple ellipse to another place with another orientation.

For tallying purposes, cell volumes and surface areas are analytically calculated for polyhedral cells and for any cell bounded by surfaces of revolution (regardless of axis of symmetry). Surfaces of revolution generally account for the majority of cells, but irregular volumes and surface areas can also be easily calculated stochastically.

A convenient mechanism is provided to specify information to be written to a file for post-processing, such as for plotting results or to generate a source for a subsequent problem.

Full restart capabilities are available that are used for machine failure or continuing a run to obtain better statistics.

Future Work

We are the first to recognize that MCNP does not do everytning for everybody. We are cautious about what goes into the code and put something in only for a good reason and after it has been carefully evaluated. However, X-6 frequently creates special versions of MCNP for the one-time requirements of special calculations or for the special requirements of a limited number of users.

The two most obvious shortcomings for use outside of Los Alamos are a lattice geometry specification and a better treatment of unresolved resonances. The lattice capability has not been of overriding importance to us at Los Alamos, but if others are interested in this feature we could be persuaded to increase the priority of it.

As mentioned earlier, we are always improving the existing variance-reduction techniques and devising new ones. We are interested in photo-neutron transport, but this is mainly a problem of data. Work is presently in progress on a three-dimensional plotter; our geometries have become so complicated it is hard to comprehend them with two-dimensional slices. Graphical techniques are being explored for post-processing of output data and for visual aids to help understand the characteristics of a problem (i.e., where are the particles going and how does a variance-reduction technique influence them). Studies of Monte Carlo vectorization are underway to see how we can take advantage of modern computer architecture (such as the CRAY-1) or future computers with parallel, independent processers.

MCNP is not a static code. It is under constant scrutiny and development by X-6. We release a new version about once a year with the current code being Version 2A. If MCNP ever becomes static, it will be so because there is no further use for it. We do not anticipate this happening; rather, the opposite seems to be the case.

MCMG

The multigroup code MCMG has basically the same features as the continuous-energy code MCNP, but it relies on the same user-supplied multigroup, multitable cross-section data that are used in discrete ordinates codes. Unlike the data for MCNP, the multigroup data treatment results in problem-dependent cross sections that can place a burden on the user to assemble and understand. MCMG can be applied to standard shielding problems, to problems in reactor physics including the use of thermal upscatter matrices, to problems in accelerator or cosmic-ray shielding at very high energies, to problems in neutral atom transport in plasmas, and to any other problem in linear transport for which multigroup data have been developed.

An added feature of MCMG is that it is also an adjoint code. A cell- and energy-dependent scalar flux is automatically generated during a forward-mode calculation, and this information is used for importance sampling of adjoint collisions and for an energy-dependent geometric splitting and Russian roulette game in the adjoint tracking.

The distribution of scattering angles for group-to-group transfer is represented by either continuous, equiprobable cosine bins or by MORSE-type discrete-scattering angles, both of which preserve all of the moments of the truncated Legendre representation.

MCMG has an advantage over discrete ordinates codes in that it does not suffer from geometrical restrictions. Like discrete ordinates codes, however, it can be limited by the approximations that are inherent in the multigroup data that can, for example, result in masking the existence of self-shielding effects.

CONCLUSION

In our opinion (admittedly biased in the true nature of Monte Carlo), Group X-6 is a very strong, experienced, and versatile Monte Carlo group. Our code MCNP is a leading Monte Carlo code because of its maturity, generality, ease of use, reliability, richness of variance-reduction techniques, documentation, cross-section libraries, and active support and development by the expertise of X-6.

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