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AUTHOR(S): John S. Hendricks

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Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

MCNP4A: Features and Philosophy

John S. Hendricks
Los Alamos National Laboratory
Los Alamos, NM 87545, USA

In this paper we describe MCNP, state its philosophy, introduce a number of new features becoming available with version MCNP4A, and answer a number of questions asked by participants in the workshop.

MCNP is a general-purpose three-dimensional neutron, photon and electron transport code. Its philosophy is "Quality, Value, and New Features." Quality is exemplified by new software quality assurance practices and a program of benchmarking against experiments. Value includes a strong emphasis on documentation and code portability. New features are the third priority.

MCNP4A is now available at Los Alamos. New features in MCNP4A include enhanced statistical analysis, distributed processor multitasking, new photon libraries, ENDF/B-VI capabilities, X-Windows graphics, dynamic memory allocation, expanded criticality output, periodic boundaries, plotting of particle tracks via SABRINA, and many other improvements.

Overview of MCNP

MCNP is a general purpose Monte Carlo code for calculating the time-dependent continuous-energy transport of neutrons, photons, and/or electrons in three-dimensional geometries. Both fixed source and k_{eff} criticality problems can be solved and a number of output tally options are available. Data representations either can be fully or partially continuous or multi-group. The code is rich in variance reduction techniques that improve the efficiency of difficult calculations. 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.

MCNP is used for many applications: nuclear criticality safety, radiation shielding, nuclear safeguards, detector design and analysis, nuclear well logging, personnel dosimetry, health physics, accelerator target design, medical physics and radiotherapy, including BNCT, PET and neutron and photon oncology, aerospace applications, radiography, waste disposal, decontamination and decommissioning, and both fission and fusion reactor design. Recent major applications at Los Alamos include nuclear criticality safety, strategic nuclear materials safeguards, accelerator transmutation of nuclear waste, accelerator production of tritium, TOPAZ reactor analysis, facilities design, health physics, space exploration, environmental science, and reactor design.

MCNP is distributed for Los Alamos by the Radiation Shielding and Information Center (RSIC) in Oak Ridge, Tennessee, and, of course, OECD/Nuclear Energy Agency (NEA) in Saclay, France. We estimate that there are a thousand active users around the world at one hundred installations.

The Monte Carlo method was developed at Los Alamos during the Manhattan Project in the early 1940s. The current MCNP code is the heir to those early efforts. About 400 person-years have been invested into the research, development, programming, documentation, and data bases for MCNP. The first multipurpose code version, MCS, was written in 1963. In the mid-70's, neutron and photon codes were merged to form MCNP, which has undergone major upgrades approximately every two to three years since. MCNP3 was released in 1983 and rewritten in standard Fortran. MCNP3A was released in 1985 and featured a very flexible generalized source. MCNP3B was released in 1988, featuring a repeated structures and/or lattice capability, a multigroup option, and tally output plotting.

MCNP4 was released in July 1990 at Los Alamos and in March 1991 to the Reactor Shielding and Information Center at Oak Ridge (version MCNP4.2). In addition to being the first MCNP specifically designed for UNIX operating systems, MCNP4 had many new features included a continuous-energy electron transport package based on the Sandia National Laboratories Integrated Tiger Series (ITS)[2], a thick-target bremsstrahlung approximation incorporated to model electron-induced photon production using the ITS electron data, shared memory multitasking, a pulse-height tally model to record energy deposition, next-event estimators for $S(\alpha, \beta)$ thermal scattering[3,4] and better random number control[5].

MCNP4A has just been released at Los Alamos (designated MCNP4XF) and should be available for international distribution next fall. New features in MCNP4A include enhanced statistical analysis[6] and distributed processor multitasking[7] which are described elsewhere at this meeting in papers by Art Forster and Gregg McKinney. Other features are new photon libraries, ENDF/B-VI capabilities, X-Windows graphics, dynamic memory allocation, expanded criticality output, periodic boundaries, plotting of particle tracks via SABRINA, and many smaller improvements.

MCNP has an active research program, some of which is described in papers by Ken Burn and Randy Baker at this meeting. Additional studies include investigations by Tom Booth in non-Boltzmann tallies[8], phase space division[9], automatic importance generation[10], angle bias, and other topics.

MCNP Philosophy

The philosophy of MCNP is "Quality, Value and New Features." The highest priority for MCNP is quality, as exemplified by new software quality assurance practices and a program of benchmarking against experiments. The second priority is what we call value, which includes a strong emphasis on documentation and code portability. New features are the third priority.

As part of the emphasis upon quality, a fairly rigorous test set and validation procedure was made available starting with MCNP4. Since then every change in the code can be traced to a specific document as part of our Software Quality Assurance Program. Furthermore, the test set has been constantly upgraded and configuration management is stricter.

A major benchmarking program has been undertaken for MCNP as a second component of the quality control program. Los Alamos has made comparison with a wide variety of neutron[11] and photon[12] experiments. A comparison of MCNP to KENO using the KENO test problem set has just been released[13]. Still more benchmarks studies have been done as collaborations in which benchmark reports are required to provide unambiguous input descriptions, specifically an MCNP input file, and are advertised and available via the MCNP E-mail network (mcnp@lanl.gov). As part of this coordinated effort, collaborators at General Electric have published light water reactor critical benchmarks[14] and collaborators at Westinghouse Idaho Nuclear Company have published several volumes[15,16,17,18] comparing MCNP to SCALE and experiments.

The "value" component of the MCNP development program includes better documentation and portability to various computer platforms. The MCNP manual is being rewritten. A primer is being written on how to use MCNP for criticality safety problems. The primer gives new users a step-by-step guide for setting up and interpreting MCNP problems starting with simple examples (critical spheres) and building up to more sophisticated problems likely to be encountered by criticality practitioners.

Also as part of "value" MCNP is maintained on many computer platforms. Actually, the source code is the same for all platforms with various portions turned on or off at compilation time. To further enhance the value of MCNP on different platforms or clusters of workstations, we have just added to MCNP4A X-Windows graphics, PVM Multiprocessing (described by Gregg McKinney in a related paper at this meeting), and dynamic memory allocation on UNIX platforms. These and other new features will now be described.

New MCNP4A Features

X-Windows Graphics: MCNP geometry and tally plotting now work with Xwindow based window systems (e.g., Open Windows, Motif, etc.) in addition to GKS, CGS, DISSPLA, and PLOT10. The X libraries are well-established and can be found on most workstations and mainframes. This capability has been tested on SUNs, IBM RS/6000s, HP, and Cray UNICOS. The graphics window can be easily resized, iconized, or printed and can be sent to or from other displays.

PVM Multiprocessing: MCNP can now be run in parallel on a cluster of workstations[7] using PVM (Parallel Virtual Machine) software. On the 16-machine IBM cluster at LANL, MCNP runs ten times as fast as a single-processor YMP. PVM multiprocessing has also been demonstrated on a network of SUN workstations. PVM multiprocessing is described in more detail in another paper by Gregg McKinney at this meeting.

Dynamic Memory on UNIX systems: MCNP now dynamically adjusts its memory to problem size on UNIX systems. The new UNIX dynamic memory manager also works in conjunction with the distributed memory multiprocessing.

A New Means of Assessing Tally Quality: MCNP4A features a new, exclusive error analysis in addition to the usual estimate of tally variance. The variance of the variance and the underlying history score probability density function are calculated and analyzed as new aids to assess tally convergence.[6] Each tally is also subjected to ten statistical checks providing new confidence and insight into the statistical convergence process. Details are given in another paper at this meeting by Art Forster.

ENDF/B-VI Physics: The Kalbach-87 formalism (ENDF/B-VI file 6 LAW=1, LANG=2) and correlated energy-angle scattering (ENDF/B-VI file 6 LAW=7) have been incorporated in MCNP to handle new ENDF/B-VI data formats. A new algorithm has been developed for next event estimators so that collisions using these laws now contribute to point and ring detectors as well as the DXTRAN variance reduction method. Preliminary libraries are available and work is proceeding to process, test, and release entirely new ENDF/B-VI libraries.

Extended Photon Libraries and Electron Options: The photon libraries have been extended to 1000 MeV based upon the Livermore Evaluated Photon Data Library (EPDL)[19].

New Criticality Analysis and Output: Since the early 80's MCNP has had three estimates of k_{eff}: collision, absorption, and track length. MCNP has also had collision and absorption estimators of removal lifetime. These are calculated for every cycle and are averaged over the cycles as simple averages and covariance weighted averages. Correlation coefficients between estimators are also calculated.

In MCNP4A the following have been added:

- a check to determine if each cell with fissionable material had tracks entering, collisions, and fission source points to assess problem sampling.

- tests for normality of the active k_{eff} values for each estimator. We believe that this is the first normality check in any major criticality production code.

- a table of k_{eff} and confidence intervals if the largest value of k_{eff} for each estimator occurs on the next cycle.

- a fission neutron lifetime estimate.
- A table of k_{eff} and its variance as it would have been calculated with a different number of k_{eff} sources per batch and with different numbers of settling cycles.

Repeated Structures Tallies: MCNP tallies can now be made in individual lattice elements or repeated cells or combinations thereof in repeated structures geometries.

SABRINA Particle Tracks: History files are now optionally output from MCNP to describe particle trajectories which can be plotted with the three-dimensional color graphics code SABRINA. This new visualization capability will provide important insight into Monte Carlo solutions.

White and Periodic Boundaries: MCNP now models both white and periodic boundaries.

Case Insensitivity: For the first time MCNP is case insensitive which is particularly of interest on VMS systems.

Easing of Column Restrictions: The old fashioned requirement of input being required in certain columns of the input file is greatly relaxed.

Answers to Specific Questions

The workshop participants have requested that a number of issues be addressed. Most questions had to do with parallel processing and automatic biasing. There were also many specific MCNP questions. Those that are not answered in the above text are now addressed here.

Vector and Parallel Processing: On an N-processor Cray or an N-node cluster of workstations, the MCNP speedup is almost a factor of N when parallel processing is used. See the PVM multiprocessing paper by Greg McKinney at this meeting. However, MCNP is seldom run in parallel on the Crays at Los Alamos because a single job uses less cpu (no overhead) and less clock time because of time sharing and scheduling problems. PVM distributed multiprocessing appears more successful.

We are looking at massively parallel archictectures, but feel that any successful commercial machines will soon look like desktop UNIX workstations with the parallelism invisible to both the programmer and user. Therefore, we do not feel it is prudent at this time to expend precious resources investigating massively parallel machines that will not resemble the machines most commonly used by our user community.

There were several questions about random number sequences for parallel processing. This is not a problem for MCNP since each history has always had its own unique random number seed.

Although vectorization has been successfully applied to special-purpose Monte Carlo computer codes, several attempts with MCNP have failed because of the code generality.

Automatic Biasing Schemes: MCNP has automatic biasing since the weight window generator was introduced a decade ago[20]. It does not yet work with electrons. Like similar schemes (see the paper by Ken Burn at this meeting) it requires user intervention and several iterations. When used correctly it can result in significant improvements in performance, but these improvements are difficult to quantitize; it can be millions of times more efficient than analog Monte Carlo, and is usually about ten times more efficient than what a skilled Monte Carlo user could do by trial and error.

Charged Particle Transport: For high energy and charged particle transport we recommend the LAHET code system[21]. MCNP does have a continuous-energy electron transport capability taken from the Integrated Tiger series of codes and MCNP also has a Boltzmann-Fokker-Planck multigroup capability so one could transport charged particles if multigroup cross sections were provided.

Input of CT-scan Data: MCNP has to be modified ("patched") to input CT-scan data efficiently. We have proposals to provide for a regular-rectangular grid geometry which would enable direct mapping of such geometries into MCNP. Experience with prototypes incidates that large grids ($>$ 1 million mesh points) perform as fast as a few hundred general MCNP cells. Financial support is required for further development.

Graphics Plans: A new version of SABRINA is being prepared and MCNP4A now writes files for particle-track plotting. We continue to investigate a general graphical user interface for setting up MCNP problems but are not yet close to having something for the user community. Attempts to link MCNP or SABRINA graphics to CAD-CAM graphics have failed mostly because the details that a mechanical engineer includes in a CAD-CAM geometry are irrelevant to radiation transport and the details needed for radiation transport are irrelevant to mechanical engineering.

How does memory allocation depend upon input? The biggest demand on MCNP memory is continuous-energy neutron cross sections followed by multidimensional tallies: each tally bin requires five or more words of memory and a tally of 100 energy bins, 100 direction cosines, 100 time bins, etc., gets very big very fast. Note that the forthcoming MCNP4A has dynamic memory allocation on all UNIX systems.

Can both TTB and electron transport be in the same problem? No. If electron transport is turned on, the thick target bremsstrahlung (TTB) approximation is turned off, even if electron importance is zero.

What About Directional Biasing? We plan to add the DXANG[22] angle biasing technique to MCNP4B. Note that the exponential transform is a fairly effective angle biasing method by itself, and that most pure angle bias methods are unstable[23].

Positron Emission Tomography We are doing PET research in collaboration with University Hospital, Cleveland. Presently we cannot have positron sources in MCNP without patching the code. Also, non-Boltzmann Monte Carlo requires an entirely new variance reduction approach. Progress is being made but will not be generally available in MCNP for years.

Whatever happened to the MCMG Multigroup code? MCMG became part of MCNP3B. MCNP now has full multigroup and adjoint capabilities.

Other comments:

- We would like to, but have no funding for, perturbation Monte Carlo;
- Presently we have no plans for improving the plotting of tori;
- We have no plans to add combinatorial geometry. Note that SABRINA will translate combinatorial geometries to MCNP and any future graphical user interface will probably handle combinatorial geometries;
- We are not considering further investigation of or generation of multigroup cross sections until ENDF/B-VI is processed. Note that Randy Baker has done some work in this area and is presenting a related paper at this meeting.
- We are presently working on a modest description of the MCNP electron physics for the new MCNP manual. Unfortunately, a detailed description of our algorithm is beyond our present resources. The MCNP

algorithm was adapted from the Integrated Tiger Series (ITS)[2] version 1. Because MCNP lags behind ITS, the only reason for using MCNP rather than ITS for electron transport is to do coupled neutron-photon-transport or because the user is already familiar with MCNP and not ITS. We believe ITS is the best electron transport code.

- MCNP has some preliminary ENDF/B-VI data for neutrons above 20 MeV, but we don't make it available. Running ANISN multigroup cross sections in MCNP is possible if someone converts the data to the proper format.

- Presently there are no plans for photon or electron transport in MCNP below 1 keV.

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