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Title: MCNP Applications for the 21st Century

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# MCNP Applications for the 21<sup>st</sup> Century

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## Abstract

The Los Alamos National Laboratory (LANL) Monte Carlo N-Particle radiation transport code, MCNP, has become an international standard for a wide spectrum of neutron, photon, and electron radiation transport applications. The latest version of the code, MCNP 4C, was released to the Radiation Safety Information Computational Center (RSICC) in February 2000. This paper describes the code development philosophy, new features and capabilities, applicability to various problems, and future directions.

## 1 Introduction

Approximately every three years, the LANL Monte Carlo Team releases a new version of MCNP for distribution through RSICC. MCNP is a general purpose, 3-D, time-dependent, continuous-energy Monte Carlo coupled neutron-photon-electron transport code. The previous version, MCNP 4B [Briesmeister, 1997], was released in February of 1997, and the new version, MCNP 4C [Briesmeister, 2000] is now available from RSICC. MCNP has become an international standard for a wide spectrum of neutron, photon, and electron radiation transport applications. These applications include nuclear reactor design, radiation shielding, nuclear criticality safety, decontamination and decommissioning, detector design and analysis, nuclear safeguards, accelerator target design, health physics, medical tomography and radiotherapy, nuclear oil well-logging, waste storage and disposal, and radiography. This paper describes the MCNP code development philosophy, new features and capabilities, applicability to various problems, and future directions. The overall development philosophy revolves around the edicts of quality, value, and features with emphasis prioritized in this order. MCNP 4C contains several new capabilities, including macrobodies, unresolved resonance treatment, alpha eigenvalue search, perturbation enhancements, superimposed mesh weight-window generator, ENDF/B-VI and electron physics enhancements, delayed neutron treatment, and parallelization enhancements. Many of the new and existing features are applied to several transport applications. Finally, the last section of the paper describes capabilities under development for the next release of MCNP.

## 2 Code development philosophy

The development philosophy for MCNP continues to revolve around the edicts of quality, value, and features with emphasis prioritized in this order. The following sections elaborate on each of these aspects.

## 2.1 *Quality*

Our quality goal is to provide a bug-free code that produces accurate results. This is accomplished primarily by our adherence to our Software Quality Assurance Plan [Abhold, 1996] which is consistent with the requirements and guiding principles found in SQA standards [IEEE, 1998; ISO, 1997]. This plan provides details of our development process, including specifics about process management controlled by a Board of Directors (BOD), documentation, standards, reviews and audits, regression testing, bug tracking, and configuration management. The MCNP regression suite gives 97% coverage of the code [Hendricks, 1996] and exact tracking is required for a successful execution. An extensive benchmarking program has existed over the past few decades (see page 21 of reference [1] for a list of references). The nearly 3000 international MCNP users provide a plethora of quality assurance inspectors who often scour the source code for physics details. Finally, we offer cash rewards as an incentive to report discovered bugs. There have been just over 100 recipients of such awards since the inception of this program with the release of version MCNP 4 in 1991.

## 2.2 *Value*

Our second development priority is value, and our goal is to provide more than just an executable. Complete documentation is of utmost importance to adding value. In addition to the 600+ page manual, we generate an average of two detailed reports each year. Most of this documentation can be accessed through our web site (<http://www-xdiv.lanl.gov/XCI/PROJECTS/MCNP>). In addition to the documentation, we distribute the source code. This benefits users not only as a means of documentation, but also through the ability to add new capabilities to the code which are often forwarded to the development team for inclusion in subsequent versions. Second in importance related to value is our adherence to ANSI standard Fortran-77 and C, making MCNP very portable. MCNP 4C is supported on everything from PCs to mainframes, including numerous operating systems (Windows 9X/NT, Linux, Sun Solaris, IBM AIX, SGI IRIX, HP HPUX, DEC Ultrix, and Cray Unicos). Additionally, we have established an international training program as a means of providing value. In 2000, seven one-week workshops were offered in the United States, United Kingdom, Germany, and Japan. Finally, MCNP also has an active research program. This program has led to such advances as the statistical analysis package and may, in the future, provide techniques for exponential convergence.

## 2.3 *Features*

Although features have a lower priority than quality and value, the MCNP development team does not neglect capability. Important standard features that have been in MCNP for many years include: (1) a powerful general source, criticality source (both  $k_{eff}$  and alpha), and surface source; (2) interactive geometry, cross-section, and tally graphics; (3) extensive input diagnostics and summary information; (4) detailed mathematical physics algorithms and associated cross-section libraries; (5) a rich collection of variance reduction methods; (6) a flexible tally structure; and (7) statistical analysis of results including detection of false convergence. In fact, since the release of version 4A in 1993, there has been an average of 5 significant new capabilities added to MCNP per year.

## 3 New features and capabilities in 4C

There are ten significant code enhancements included in the release of MCNP 4C. These are highlighted in the following sections.

### *3.1 Macrobodies*

MCNP has always had a fully 3-D surface-sense geometry that is capable of modeling any space bounded by 1<sup>st</sup> and 2<sup>nd</sup> degree surfaces (conic sections) and 4<sup>th</sup>-degree elliptical tori. These geometries are general and flexible, but also can be complex and difficult to describe. Macrobodies are groups of surfaces that mimic combinatorial geometry bodies like those used in the Integrated Tiger Series [Halbleib, 1992] and other 3-D Monte Carlo codes. Macrobodies supported in version 4C are BOX, RPP (right parallelepiped), SPH (sphere), RCC (right circular cylinder), and RHP or HEX (right hexagonal prism). These macrobodies can be used in combination with all the former MCNP surfaces to more easily construct complex geometries. Other macrobodies (REC, ELL, TRC, etc.) will be included in the next version of MCNP.

### *3.2 Unresolved resonance treatment*

MCNP 4C improves upon the already first-rate, continuous-energy neutron physics package by adding unresolved resonance range probability tables [Carter, 1998; Mosteller, 1999]. The statistical treatment of unresolved resonances improves intermediate energy spectrum neutron problems whenever neutron self-shielding is important. In particular, it can make significant differences in the calculation of certain criticality eigenvalue problems.

### *3.3 Superimposed mesh weight windows*

A significant advance has been made in MCNP variance reduction with the new superimposed importance mesh and weight window enhancements [Evans, 1998]. Before version 4C, users had to subdivide geometries sufficiently well to specify importance functions for variance reduction. Simple problems that can be described with a few dozen geometric cells often required hundreds of cells to specify smoothly changing importances or weight windows. Now the simple geometry can be specified with an importance mesh superimposed in either rectangular or cylindrical geometry. Furthermore, the weight window generator technique of MCNP may be used so that the code will determine the optimum importance function for the superimposed mesh. An assessment [Culbertson, 1999] of the revised weight window capabilities added in MCNP 4C indicated that (1) MCNP 4C utilized weight windows comparably to MCNP 4B, but (2) generated cell-based weight windows 50% better than 4B, and (3) that superimposed mesh windows could be superior to cell-based windows and eliminate the need to subdivide geometries for importances.

### *3.4 Delayed neutron physics*

A time-dependent delayed neutron treatment provides a more accurate fission model in fixed-source and criticality calculations. A natural sampling of prompt and delayed neutrons is now the default for eigenvalue problems. This capability is also available to users for fixed-source problems. Furthermore, a delayed neutron biasing scheme is available due to the low probability of a delayed neutron occurrence.

### *3.5 Alpha eigenvalue*

MCNP 4C also includes an alpha (time) eigenvalue search, in addition to the  $k_{\text{eff}}$  criticality eigenvalue. The alpha eigenvalue describes the asymptotic time evolution of the system containing fissile materials when the neutron population depends upon time as  $e^{\alpha t}$  [Bell, 1970]. Alpha may

characterize a subcritical ( $\alpha<0$ ), critical ( $\alpha=0$ ), or supercritical ( $\alpha>0$ ) system. MCNP can find either positive or negative alpha values. The method imposes alpha as an  $\alpha/v$  interaction term, where  $v$  is the neutron velocity. For  $\alpha>0$ , this term is a time absorption. For  $\alpha<0$ , this term is an (n,2n) time creation. The alpha values are then iterated to achieve  $k_{\text{eff}}=1$  following the prescription of reference [2].

### *3.6 Electron physics upgrade*

Several electron physics improvements are included in MCNP 4C. Most notable, the radiative stopping powers have been upgraded to the Seltzer model in ITS 3.0 [Halbleib, 1992]. The ITS 3.0 density correction and bremsstrahlung production models have been added. Variance reduction has been enhanced to improve the sampling of photons produced from a bremsstrahlung event. Finally, the fluorescence and k x-ray relaxation models in MCNP have been made more self-consistent.

### *3.7 Perturbation enhancements*

MCNP 4B featured a differential operator perturbation capability so that small changes in problems could be modeled in a single calculation rather than having to compare the statistically noisy results of separate runs. However, a laborious correction had to be made [Densmore, 1997] for determining perturbations to  $k_{\text{eff}}$  and reaction rate tallies involving cross sections. In MCNP 4C, the perturbation technique has been upgraded to enable perturbations of cross-section dependent tallies [Hess, 1998]. Now the perturbed values of  $k_{\text{eff}}$  are automatically printed for each perturbation, and cross-section dependent tallies work with perturbations without further adjustments.

### *3.8 Parallelization improvements*

In MCNP 4C, the ability to compute on massively parallel platforms has been enhanced. While previous versions have supported distributed-memory multiprocessing (DMMP) and shared-memory multiprocessing (SMMP) separately, version 4C allows for the simultaneous use of these capabilities. DMMP message passing is still invoked with PVM [Geist, 1993] and SMMP threading is invoked through compiler directives. The next version of MCNP will support DMMP with MPI (<http://www-unix.mcs.anl.gov/mpi>) and SMMP with OpenMP (<http://www.openmp.org>). By combining shared memory threading with distributed memory multiprocessing, most MCNP calculations can be run efficiently on large numbers of processors for high throughput. Efficiencies exceeding 90% have been obtained at LANL, even when executing across thousands of processors.

### *3.9 ENDF/B-VI upgrade*

The nuclear data sampling routines were modified in version 4C to enable utilization of the ENDF65 neutron data library. Tabular-angular sampling distributions are added to the MCNP ACE (A Compact ENDF) format for representing angular information in finer detail than through the 32 equi-probable bin distributions. Furthermore, neutrons and photons are now handled consistently within the energy-sampling portion of laws 4, 44, and 61, which use emission-energy tables. Finally, nearest integer syntax is used to correct problems when using single-precision data to carry large pointers.

### *3.10 PC enhancements*

MCNP 4C can now compile on PCs with Fortran 90/95 using either Lahey (<http://www.lahey.com>) or Digital Visual Fortran (DVF, <http://www.digital.com/fortran>) compilers. Plotting is available with an X-window interface using either compiler, or optionally with regular Windows using Lahey's Winteracter package or DVF's QuickWin plotting package.

## 4 Transport applications

MCNP applications span more than a dozen nuclear related fields. The following sections discuss the importance of various MCNP 4C features to four such nuclear applications.

### 4.1 Reactor application

Reactor problems, like the BWR octant shown in Figure 1, demonstrate the repeated structures (e.g., lattice) capabilities that have been present in MCNP for many years. Up to ten levels of embedded universes can exist in a single input, and the MCNP geometry plotter is now able to plot any one of these levels. Recent physics enhancements important to these types of applications include unresolved resonance and delayed neutron treatments. Neither have been shown to have a significant impact on most applications, however there is little doubt that some applications will benefit from these physics improvements. Algorithm enhancements relevant to criticality problems include an alpha eigenvalue search and an automatic perturbation output. This latter feature greatly simplifies perturbation and sensitivity analyses.

### 4.2 Medical application

Radiotherapy problems, like the BNCT (Boron Neutron Capture Therapy) simulation depicted in Figure 2, require the transport of millions and even billions of particles for high-resolution calculations. Parallelization enhancements available in MCNP 4C make such simulations possible.

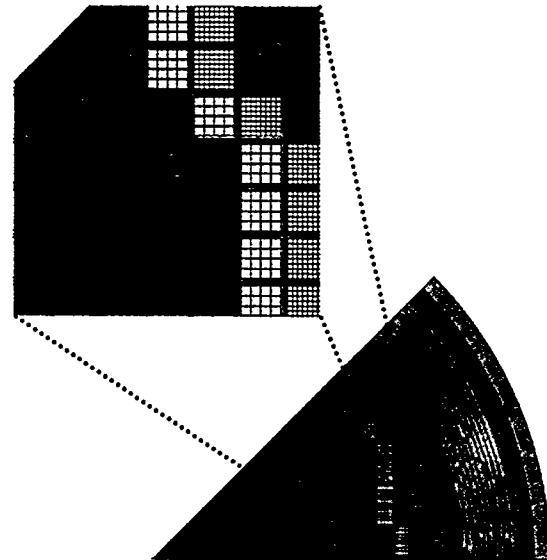


Figure 1. Octant model of a BWR with an expanded view of several fuel bundles.

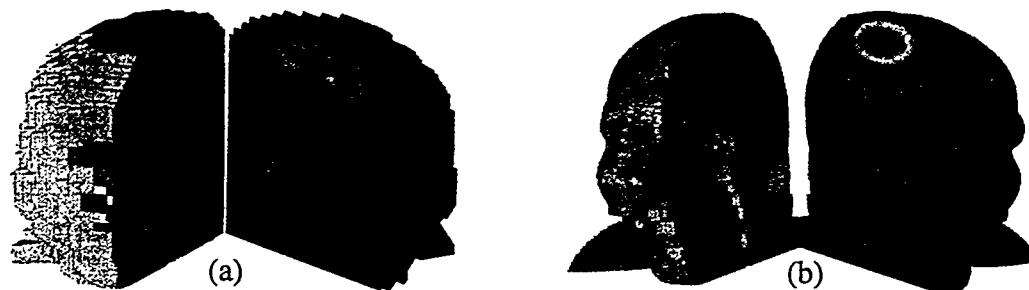


Figure 2. Left half of head shows the MCNP 3-D lattice material input from a CAT scan. Right half of head shows dose contours for 1 cm (a) and .5 mm (b).

Figure 2(b) shows energy deposition contours calculated on a 0.5 mm mesh using all 6144 processors of the ASCI Blue Mountain computer. Note the facial features that become obvious with this fidelity compared to Figure 2(a) which presents contours for a typical 1 cm simulation. High parallel efficiency is achieved by the use of threads within a shared-memory unit and the use of message-passing across distributed-memory units. Furthermore, many medical and dosimetry applications will benefit from the electron physics enhancements provided in 4C.

#### 4.3 Oil-well logging application

Detector problems, such as the oil-well logging neutron porosity tool model shown in Figure 3, are now much easier to set up in MCNP 4C. Such geometries can now be specified using a handful of macrobodies (BOX, RPP, RCC, etc.), and the numerous material subdivisions needed to apply variance reduction techniques (e.g., weight windows) are no longer necessary. With the addition of 2 MCNP 4C input cards (WWG and MESH), one can specify a rectangular or cylindrical mesh upon which weight-window parameters will be estimated. In a subsequent run, this mesh weight-window information can be used to "steer" particles toward the tally region, greatly reducing the variance of a tally. In assessing this mesh weight-window capability [Culbertson, 1999], it was found that for most applications this technique outperforms skillfully developed cell-based windows and significantly reduces user setup time.

#### 4.4 Accelerator application

Accelerator and shielding problems, such as the LANSCE (Los Alamos Neutron Science CEnter) accelerator neutron production simulation shown in Figure 4, will also benefit from several MCNP 4C improvements. Not only can the mesh weight-window generator be used to significantly increase tally convergence while eliminating the need for material subdivisions, parallel enhancements allow for the transport of millions of particles per minute using workstation clusters or massively parallel computers. Additionally, MCNP 4C upgrades in the ENDF/B-VI cross-section physics produce higher fidelity results.



Figure 3. Left figure shows an axial cut through a neutron porosity tool model with the smaller near and larger far detectors. Right figure shows a perpendicular cut through the near detector and displays the tool placement against the borehole wall.

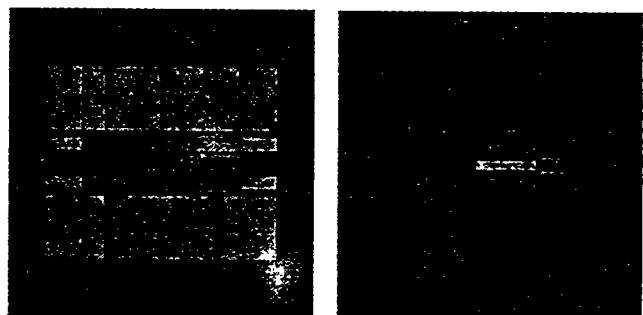


Figure 4. Left figure shows an axial cut through an accelerator Pb target model. Also shown is the surrounding Pb blanket and  $\text{MnSO}_4$  bath. Right figure shows a similar model for a W target.

## 5 Future development

In October 1999, the LANL Monte Carlo Team was moved into the newly created Diagnostics Applications Group of the Applied Physics Division. Furthermore, MCNP principal support is now funded through the Eolus project of the DOE Accelerated Strategic Computing Initiative (ASCI, <http://www.lanl.gov/ASCI>) program. These changes will have little impact on the future research and development related to MCNP and are likely to result in an increased interest in adaptive Monte Carlo, code modernization, and charged particle transport.

### 5.1 Adaptive Monte Carlo

LANL has teamed with the Claremont Research Institute of Applied Mathematical Sciences (CRIAMS, <http://criams.cgu.edu/>) to investigate adaptive Monte Carlo methods. This collaboration is in its fifth year and has made significant progress in demonstrating geometric convergence on 1,2-D problems. The two approaches being investigated are Adaptive Importance Sampling (AIS) and Sequential Correlated Sampling (SCS). The AIS method involves establishing zero-variance continuous importance functions by estimating infinite series expansion coefficients [Booth, 1998, 1999]. The SCS method achieves geometric convergence by estimating expansion coefficients for correction terms generated from a reduced source iteration [Spanier, 1999].

### 5.2 Code modernization

In 1999, a software engineering assessment was performed by the ASCI program. Our SQA process received an average SEI (<http://www.sei.cmu.edu/>) rating of 4 on level 2 and 3 key process areas. This rating puts us in the 80-90<sup>th</sup> percentile of international code development projects. As a result of this assessment, The Monte Carlo Team is in the process of implementing the Razor (<http://www.tower.com>) software engineering tool. Once implemented, this tool will formalize the process of code modifications and documentation, provide bug tracking and automatic regression testing, and generate required SQA reports for the release of new code versions. Finally, our modernization plans include an upgrade from Fortran 77 to Fortran 90. This will result in gradual, yet significant, changes to MCNP data structures, memory management, and code structure.

### 5.3 Charged particles

The MCNPX code project [Hughes, 1998], which is organizationally separate from the MCNP development effort, has successfully merged MCNP 4B and the LAHET codes into a new research code for the Accelerator Production of Tritium program. MCNPX is capable of transporting over 30 different particles and offers a variety of high-energy physics packages. The Monte Carlo Team is in the process of integrating numerous MCNPX capabilities into MCNP, starting with a proton physics package. This will be a multi-year effort which will eventually converge these capabilities into a single code.

## 6 Conclusions

For the past 35 years, MCNP has provided important modeling and simulation capabilities for radiation transport. The emphasis in methods and code development has been on quality first, followed by value and features. Many significant code enhancements have been added to MCNP 4C which is currently available. Many more exciting advances are under development that will increase

the ease of MCNP use while expanding the classes of radiation transport problems that can be solved as we move into the 21<sup>st</sup> century.

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