MCNP Version 5

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INTRODUCTION

MCNP [1] is a well-known and widely used Monte Carlo code for neutron, photon, and electron transport simulations. For the past year, an intensive effort to modernize MCNP has been carried out by the Monte Carlo Team at LANL. The result of this effort is Version 5 of MCNP.

MCNP was first released in the mid-1970s for neutron and photon transport, and was enhanced over the years to include generalized sources and tallies, K-effective eigenvalue calculations, volume calculations, electron physics and coupled electron-photon calculations, interactive plotting of geometry and tallies, cross-section plotting, repeated structures and lattice geometry, parallel processing, perturbation theory, detectors and pulse height tallies, automated weight window generation, many variance reduction options, an unresolved resonance treatment, macrobody geometry, statistical convergence tests, and many other user-requested features. The code is supported by a detailed 800-page manual, a series of application classes, and an extensive verification/validation effort. It is estimated that there are approximately 300 MCNP users at LANL and over 3,000 users worldwide. The previous version of MCNP, Version 4C2, was released in 2001. As for many other large, mature, production-oriented code systems, the evolution of the coding itself has lagged the very rapid changes in computer hardware and software technologies. Coding style, Fortran language features, version control, issues tracking, compilation/installation procedures, etc., were based on 1970s practices. Rigid adherence to these practices served to maintain high code quality over the years, but has increasingly impeded further advanced development. With the advent of the DOE Accelerated Strategic Computing Initiative (ASCI), there has been significant focus on upgrading the software development and quality assurance practices at DOE laboratories, to ensure that codes can fully utilize the ASCI teraflop computers and can be enhanced to incorporate more advanced physics modeling.

MODERNIZATION OF MCNP

The effort to modernize MCNP was driven by the need to provide for:

1. Adoption of modern practices for software engineering (SE) and software quality assurance (SQA),

2. Strict adherence to current standards for Fortran-90 and parallel processing,

3. Preservation of all existing code capabilities,

4. Flexibility for rapid introduction of new features and adaption to advanced computers.

An evolutionary approach to MCNP modernization was followed to minimize the chances of the introduction of new errors.

SE and SQA

MCNP development adheres to the software engineering requirements established for the LANL ASCI program [2] and to a new MCNP SQA plan [3]. All source coding, test problems, documentation, Unix scripts for compilation, *makefiles*, etc., have been placed under strict, formal, version control. We currently use the Razor™ system to provide for centralized source code management and version control. Files are checked-out, modified, and then checked-in, with Razor managing versions of individual files and associating a set of files with each code release. Razor is also used for issues management, associating issues with each code release. The MCNP modernization has proceeded in a series of small steps. For each step, a new thread in the version control system was produced and thoroughly tested. To date, over 50 threads have been produced.

The entire installation and test process has been revised to use the GNU *make* utility [4]. Simple configuration files are used to specify system-dependent features (e.g., compiler, libraries, optimization controls, etc.). The *makefile* includes targets for building the executable, running a set of standard installation tests, and installing the code. The source coding has been split from one very large monolithic file into roughly 330 separate files containing individual subprograms or modules. The combination of these two changes allows for very fast incremental compilations when small changes are made to the source coding. Code revisions can be distributed using the GNU utilities *diff* and *patch*, which are available for all systems, including PCs. This new build system has been used on a wide variety of computer systems, including Sun, SGI, Compaq, HP, IBM AIX, PC/Windows, PC/Linux. For PC/Windows, a Windows installer is also provided that installs a pre-compiled executable, the User Manual, the installation test set, and necessary scripts.

Standards for Fortran-90 and Parallel Processing

Every line of coding was reworked under formal version control to provide strict compliance with ANSI-standard Fortran-90. This conversion will aid in the long-term viability of MCNP, since Fortran-77 compilers are becoming obsolete. A consistent style was adopted to enhance readability and understanding of the coding. Modern Fortran-90 language features have been used to upgrade much of the coding, resulting in simplified code flow logic, a greatly reduced number of GOTO statements, encapsulation of selected features in modules, and much more readable, understandable coding. All source coding was changed to free-format Fortran-90; "comdecks" were converted to Fortran-90 modules; dynamic arrays are now constructed using Fortran-90 *allocate* statements; computed GOTOs were replaced by *case* statements; very many GOTOs were eliminated through the use of structured *if-else-endif* constructs; DO-loops were changed to eliminate shared terminations, and invoke cycle and exit statements; Hollerith usage was eliminated. To improve code readability, a consistent indentation style was applied to DO-loops, *if*

statements, and *case* statements; very many blank lines were inserted; inline comments were used where appropriate. To encapsulate and consolidate related routines and data, Fortran-90 modules were created for random number generation, OpenMP parallelism, message-passing, criticality, geometry plotting, and tally plotting. A large portion of this conversion was accomplished using specially developed tools (e.g., *perl* scripts) to ensure consistency and error-free conversion. For manual changes, the use of the Razor version control and frequent testing served to (nearly) eliminate errors, and to quickly identify and resolve the inevitable errors that did occur.

MCNP 5 is required to execute on many different varieties of parallel computer systems. To achieve parallelism in a portable manner, we rely on strict adherence to the MPI standard for message-passing (for distributed-memory parallelism) and the OpenMP standard for threading (for shared-memory parallelism). MCNP 5 can execute sequentially (no parallelism) or in parallel using only MPI message-passing, using only OpenMP threads, or using both MPI and OpenMP. In addition, we continue to support PVM message-passing (in place of MPI, primarily for heterogeneous clusters of workstations). For small calculations, we generally run MCNP 5 sequentially or with a moderate number of OpenMP threads (typically 4 or 8). For larger calculations, MCNP 5 has been run using 1000s of processors and combined MPI/OpenMP, with excellent parallel speedups.

Preservation of All Existing Code Capabilities

All previously existing code capabilities have been preserved, including physics options, geometry, tallying, plotting, cross-section handling, etc. Tally results from MCNP 5 are expected to match the tally results of problems that can be run with the previous MCNP 4C3, except where bugs were discovered and fixed in the conversion process. Changes in the format and presentation of some of the printed output are allowed, but the tally results (*mctal* files) are required to match 4C3 results in all installation/regression tests. All user input files that were used with previous versions should still work; no changes to input are required for using MCNP 5 except to utilize new features.

Flexibility for New Features and Advanced Computers

One of the goals in MCNP modernization was providing flexibility for adding new features and adapting to advanced ASCI computer systems. This goal has been demonstrably met: Many new features have already been introduced into MCNP 5, as described in the next section. Recently, the same version of MCNP 5 that is used on PCs, Unix workstations, and the SGI Origin-2000 was installed and successfully tested on: a PC cluster using either MPI or PVM, the 3-Teraflop ASCI Blue Mountain system, the 12-Teraflop ASCI Blue Pacific system, and the 30-Teraflop ASCI Q system (using only 1/3 of the system – installation of the remainder is in progress).

NEW FEATURES IN MCNP 5

While a large amount of effort has been focused on modernization of MCNP, a number of new features have been developed for Version 5, including:

- Plotting enhancements: Improvements have been made to the geometry and tally plotting, with more colors and smooth gradients for shading.

- Doppler broadening for photon cross-sections: This capability is important for low-energy photon transport. Past versions of MCNP have neglected the pre-collision motion of the electron. MCNP 5 now includes the capability to handle this low-energy correction.

- Radiography tallies: Neutral particle radiography tallies [5] have been added to support neutron and photon imaging simulations. This feature uses multiple point detectors to determine the particle flux at pixel locations in a user-defined grid. As many detector points as desired can be used to create both the direct (unscattered) and scattered flux image contributions. Each source and collision event contributes to all detectors, resulting in a smooth image. Radiography simulations have been run using millions of detector points.

- Generalized source options: Enhancements to sources provide source description options that are especially appropriate to accelerator beam applications, including options to select from Gaussian spatial distributions, transformation and replication of a defined source, user selection of the type of source particle for surface sources, and built-in spectra for selected radioisotope photon sources.

- Variance reduction: Time-dependent importances can now be specified to allow varying splitting and Russian roulette parameters with time. The capability can be used for all particle types and is fully integrated with both implicit absorption and weight windows. This capability has been successfully tested on several problems where it is important to have good flux estimates at late problem times.

- Variance reduction: Pulse-height tallies are non-Boltzmann in nature because they involve collections of particle tracks. For example, an annihilation event in a detector producing two 0.511 MeV photons results in a 1.022 MeV pulse, not two 0.511 MeV pulses. The "F8" pulse height tally in previous versions could not be used with any variance reduction techniques except source biasing because of this collective nature. In MCNP 5, the "history deconvolution approach" [6] is used with pulse height tallies for photons so that additional variance reduction techniques may be applied, including geometry splitting/roulette, weight windows, exponential transform, forced collisions, energy/time splitting, some of the weight cutoffs, and *dxtran*. This has been implemented for photon-only problems (i.e., *mode:p*).

- Random numbers: In addition to modernizing the coding of the random number generator, the basic algorithm for random number generation has been extended [7]. This work has lengthened the period of the random number sequence by a factor of $\sim 10^5$, from $\sim 7 \times 10^{13}$ to $\sim 9.2 \times 10^{18}$. The increase in period is important, given today's faster computers, since it is becoming common to run problems involving $\sim 10^9$ histories, with a stride of $\sim 10^5$ random numbers allocated per history. Such calculations exceed the period of the previous random number generator, resulting in wrap-around in the random sequence and reuse of some random numbers. For MCNP 5, the default random number generator is identical to the previous one (to provide backward compatibility), but the extended-period generators may be optionally selected.

All aspects of incorporating the modernization changes and new features have proceeded on schedule. The beta-test version of MCNP 5 has been used at LANL by friendly users and in MCNP classroom instruction since January 2002. Extensive testing and final verification/validation calculations are scheduled for the summer/fall of 2002.

NEW MCNP NUCLEAR AND ATOMIC DATA LIBRARIES

In a separate but closely related effort, the Data Team at LANL will release new data libraries containing updates from the ENDF/B-VI.6, ACTI, and EPDL97 libraries. The ENDF66 library, a follow-on to ENDF60, will include data for 173 nuclides from ENDF/B-VI release 6. (ENDF60 included 122 nuclides from ENDF/B-VI release 2.) There are 58 new nuclides, and another 40 have significant updates. All of the nuclides were processed with tighter tolerances and include recent new features, where appropriate, such as unresolved resonance probability tables, delayed neutron time and energy spectra, charged-particle production data, and tabular angular distributions. ENDF66 subsumes the many special purpose libraries (ENDF6DN, URES, and LA150N) released since ENDF60. The ACTI research effort sought to provide more detailed neutron-induced photon spectra for prompt gamma-ray spectroscopy. These updated photon spectra are now included in ENDF/B-VI as part of release 8, and the 41 nuclides updated have been processed into the special purpose ACTI library. The latest LLNL photon and electron data (EPDL97, EEDL97, and EADL97) have been included in ENDF/B-VI as part of release 8. The improved photoatomic interaction cross-sections and fluorescence data will be available in a new library. Future code updates will enable better sampling of the fluorescence data to more accurately reproduce atomic relaxation.

FUTURE WORK

The release of MCNP 5 will provide the foundation for many planned improvements and new features. Some of these include:

- Superimposed mesh-based tallies: Work is in progress to provide for tallying on a user-specified mesh. As for the superimposed mesh for weight windows, the tally mesh will be independent of the problem geometry.

- Setup and visualization: We are providing support for the MCNP Visual Editor (VISED) developed by R. Schwartz and L.L. Carter, which provides a convenient GUI-based means of preparing input and visualizing geometry.

- Criticality calculations: These planned features fall into two categories, source convergence and correlation corrections. Research has been underway to develop procedures for testing the stationarity of the source distribution in K-effective calculations. That is, has the source distribution fully converged before tallies are begun? Promising results have been obtained from performing statistical tests on the Shannon entropy of the source distribution [8]. Concerning correlation corrections, it is well known that intergenerational correlation causes underprediction of the confidence intervals in Monte Carlo K-effective calculations. When correlation can be detected, the confidence intervals

should be increased to account for correlation effects. Promising results in this area have been obtained using autoregressive fitting [9].

- Variance reduction: The enhancements to pulse-height tallies, which account for variance reduction will be extended to include pulse-height tallies for electrons and coupled photon/electron modes.

- Parallelism: The parallel algorithms in MCNP 5 will be enhanced to work more efficiently. This work involves simplifying the message-passing, using some MPI collective operations, and reducing the use of OpenMP locks.

- Modernization: Additional modernization of the code is planned to include further consolidation into modules, use of Fortran-90 defined types to handle complex data structures, more understandable naming of variables, etc.

- Physics: Improvements are planned for low-energy coupled photon-electron transport, including the modeling of atomic relaxation.

- Variance reduction: Recursive Monte Carlo techniques for estimating importance are partially in place. This work will be completed to provide an alternative method for the automatic generation of weight-window parameters. In addition, the use of adjoints from deterministic calculations will be supported.

- Random numbers: The new random number generator in MCNP 5 can be readily modified to provide independent random number streams for each distinct type of particle. This capability would permit, for example, reproducibility of results for neutrons regardless of whether coupled neutron-photon physics was switched on or off. This capability would greatly extend the range of problem types for which correlated sampling is applicable.

- Particle types: Work is underway to incorporate continuous-energy proton physics and transport into MCNP 5.

In addition to the code development work described above, the MCNP developers will continue to provide MCNP classes on basic and advanced usage of MCNP, and on specialized topics such as criticality calculations, medical applications, and variance reduction.

CONCLUSIONS

MCNP 5 continues the development of Monte Carlo methods for particle transport in the same tradition as its predecessor versions over the past 30 years. Modernization of the code and incorporation of new features position MCNP 5 well for continued development and applications. MCNP 5 is a state-of-the-art Monte Carlo code, very rich in physics and geometry capabilities. The code is available through the RSICC code center.

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