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MCNP™ Version 5

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SUMMARY

The Monte Carlo transport workhorse, MCNP,[1] is undergoing a massive renovation at Los Alamos National Laboratory (LANL) in support of the Eolus Project of the Advanced Simulation and Computing (ASCI) Program.

MCNP[a] Version 5 (V5) (expected to be released to RSICC in Spring, 2002) will consist of a major restructuring from FORTRAN-77 (with extensions) to ANSI-standard FORTRAN-90[2] with support for all of the features available in the present release (MCNP-4C2/4C3). To most users, the look-and-feel of MCNP will not change much except for the improvements (improved graphics, easier installation, better online documentation). For example, even with the major format change, full support for incremental patching will still be provided.

In addition to the language and style updates, MCNP V5 will have various new user features. These include improved photon physics, neutral particle radiography, enhancements and additions to variance reduction methods, new source options, and improved parallelism support (PVM, MPI, OpenMP).

I. Modernization of MCNP

As computers, computer languages and computer science have evolved, it is become apparent over time that MCNP would have to evolve as well. Planning and implementation for this modernization has been in progress for the last two or so years.

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[a] MCNP is a trademark of the Regents of the University of California, Los Alamos National Laboratory

An important requirement of the modernization is that backwards compatibility be required. That is, MCNP 5 is expected to match the tally results of problems that can be run with MCNP 4C3 except where bugs are discovered and fixed in the conversion process. Changes in the format and presentation of some output file contents is allowed, but the tally results (mctal files) are required to match 4C3 results in all regression tests unless deviations are justified.

A. Conversion to FORTRAN 90

The major portion of the modernization effort is focused on conversion from FORTRAN 77 (with extensions) to ANSI-Standard FORTRAN 90. This conversion will aid in the long-term viability of MCNP as FORTRAN 77 compilers become obsolete. FORTRAN 90 also allows for a more-modular approach that aids in component testing, code maintenance, code reuse and addition of new features.

The MCNP Team developed an internal standard[3] for this conversion that included the following major points:

- Conversion to free-format FORTRAN 90
- Conversion of COMDECKs to data modules
- Conversion of preprocessor directives to C preprocessor format
- Conversion to FORTRAN 90 dynamic memory
- Reduction of GOTO usage
- Conversion to FORTRAN 90 logical operators
- Do-loop changes
    - END DO termination
    - Insertion of CYCLE and EXIT statements
    - Removal of shared terminations
    - Naming of long do-loops
- Creation of functional modules for
    - Random numbers
    - OpenMP parallelism
    - Distributed memory parallelism (MPI/PVM)
    - Criticality
    - Geometry Plotting
    - Tally Plotting

Other conversions include:

- Comment conversion: leading “c” to “!”
- Conversion of Hollerith to quoted strings
- Continuation line conversion
- Removal of line identifiers
- Expansion of various keywords
- Elimination of statement functions
- Overall indentation for clarity

A large portion of this conversion was accomplished through the use of specially developed tools to ensure the full conversion of all cases. Following the automated conversion, a full review and testing was performed prior to the start of the continued development of functional modules and new code features.

B. Build and Installation System Upgrades

In addition to migrating to modern FORTRAN, we have also updated the method of building MCNP to use GNUMake.[4] The source code has also been split from the one big file into many files at package (‘deck’) boundaries. The combination of these two changes allows for very fast incremental compilations when small changes to the source code are made.

For PC-Windows, a Windows Installer is provided that installs a pre-compiled executable, the User Manual[1], the installation test set, and necessary scripts. For PC-Windows users who need to compile MCNP, GNUMake is easily obtained and special files are provided to work with the supported compilers directly.

C. Modified Patching Method

In the past, MCNP patches were manually written in a custom format and applied with a custom utility (PRPR) distributed as part the MCNP package. This patch-feature relied on the presence of the MCNP line-identifiers that tagged each source code line uniquely. Since the method was specific to MCNP and the line identifiers have been dropped, a new method has been developed for providing incremental fixes and enhancements.

The new method is centered on using commonly available GNU[4] tools: *diff* and *patch*. These are available on most Unix systems and are readily available for PC-Windows systems as well. Patches are generated by using the *diff* utility and applied with the *patch* utility.

Full details for acquiring and using these utilities and future MCNP patches will be in the Users Manual[1] and posted on the MCNP website.[5]

II. New Features in MCNP V5

While a large amount of effort has been focused on modernization, there are new features in MCNP V5, too. The following sections describe some of these new features.

A. Plotting Color Enhancements

A frequent request over the last two years has been to provide a larger number of colors for plotting. In MCNP V5, there are 64 colors available for plotting geometries and tallies. This color map is arranged in an order to provide significant contrast between colors that are adjacent in the list. As in earlier versions, the colors are automatically selected based on the material index, but any color can be assigned to a specific material. The names of the available colors can be displayed by the plotter command "*options*."

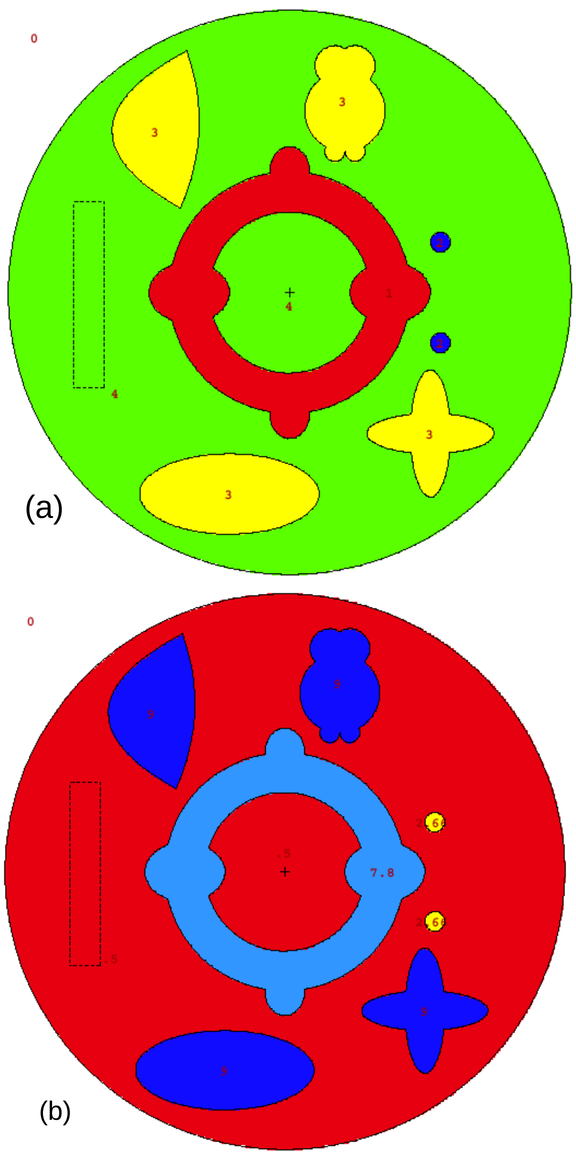

Figure 1. Geometry plots shaded by (a) material index and (b) by density. Atomic density and temperature can also be used for shading.

There is also a second set of 64 colors arranged in a smooth gradient that can be used to shade geometry plots by physical properties. At this time, density (g/cc), atomic density (atoms/cc) and temperature (MeV) can be used to color the geometry. This feature is turned on by the extension to the geometry plotter command "*color by <property>*" where *<property>* is one of (*den, rho, tmp*).

An example of the difference between shading by material index or by density is given in Figure 1.

B. Doppler Energy Broadening for Photon Transport

Incoherent scattering is an important interaction mode for low-energy photons. Past versions of MCNP have neglected the pre-collision motion of the electron in treatment of this phenomenon. MCNP V5 now includes the capability to handle this low-energy correction. The details of this work will be presented in a future ANS paper.

C. Neutral Particle Radiography

A neutron and photon radiography imaging capability has existed for MCNP for over six years.[6] Additional enhancements have been made by E. C. Snow for MCNPX.[7] This capability has been reviewed, slightly modified, and incorporated into MCNP V5 for neutron and photon imaging applications

The method 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.

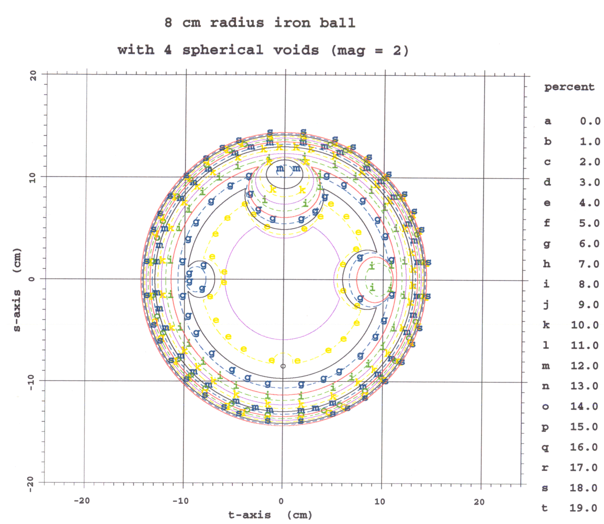

Figure 2. A radiograph of an iron ball with four internal voids.

An example of a photon radiograph is shown in Figure 2. The object is an 8cm iron ball with 4 varying size internal voids arranged in a plan orthogonal to the beam direction.

D. New Source Options
MCNP V5 provides a variety of new source options.

1. Generalized Source Options: These source enhancements provide source description options that are especially appropriate to accelerator beam applications.[8] They include new SDEF options and a generalization of an SSR option:

- SDEF: Allow a Gaussian probability distribution option for x,y,z position;
- SDEF: Allow a transformation (TR=n) or distribution of transformations (TR=Dn) to be applied after particle coordinates are sampled;
- SSR: The use of the (TR=Dn) option has also been generalized to match its extended function on the SDEF card.

2. Radioactive Source Option: The planned inclusion of a radioactive source option in MCNP V5 is an adaptation of a feature that has been in use at LANL for quite a while[9] (originally an extension to MCNP 3A). This feature allows the user to specify concentrations of photon-emitting radioisotopes instead of having to provide the details of the photon source distribution explicitly.

E. Variance Reduction: Time Importances
Version 5 has a new capability to define time importances in continuous energy transport problems. A new TSPLT card - similar to the existing energy importance ESPLT - has been added to allow particle control by time splitting and/or Russian roulette. The capability can be used for all particle types and is fully integrated with both implicit weight capture and weight windows. The ESPLT capability has also been improved to be correctly integrated with implicit weight capture. A new Print Table 80 has been created to list both energy and time importance parameters input by the user. Additional error messages have also been provided for incorrect ESPLT and TSPLT input. This capability has been successfully tested on several problems where it is important to have good flux estimates at late problem times.

F. Variance Reduction: Pulse-height Tally Enhancements
Pulse-height tallies are non-Boltzman because they involve collections of particle tracks. For example, an annihilation event in a detector (two 0.511MeV photons) results in a 1.022MeV pulse, not two 0.511 MeV pulses.

The pulse height tally in MCNP 4C2 (the "F8 tally") could not be used with any variance reduction techniques except source biasing because of this collective nature. Coding has been added to MCNP V5, based on the "*history deconvolution approach*",[10] to enable many additional variance reduction techniques with the pulse height tally.

Because of the complexity of the electron transport algorithms, the first implementation of the pulse height tally variance reduction will be for photon only (*mode:p*) problems. The specific techniques under consideration are (modifications of):

- Geometry splitting/roulette
- Weight windows
- Exponential transform
- Forced collision
- Energy/time splitting
- Some of the weight cutoffs (not all make sense for f8)
- Dxtran

G. Parallel Processing Support
MCNP Version 5 adds the support for MPI[11] for distributed parallel processing. MPI will be the best choice on homogeneous UNIX/Windows clusters or clusters of SMPs (shared-memory multi-processor computers). PVM[12] is still supported and is expected to be better for use on heterogeneous clusters.

Shared-memory parallel processing has been improved by the adoption of OpenMP[13] as the threading paradigm. OpenMP threading can be used with either MPI or PVM to provide mixed-mode parallelism. The MPI/OpenMP combination is now in regular use at the 1000+ processor level in support of the ASCI Program.

In all parallel modes, the tally answers are expected to (and mostly do) match answers from a sequential run to within round off.

III. Software Engineering
This release of MCNP is accompanied by the adoption of software engineering requirements[14] and a revised software quality assurance plan.[15] These plans and requirements address the many aspects of software engineering that are applied to MCNP.

IV. Future Work
This release of MCNP V5 will not be an endpoint. Many more enhancements and modernizations are in the planning and development stages. Some features planned for future releases include:

- Recursive Monte Carlo: A method of improving weight-window generation;
- Superimposed mesh-based tallies: An option being adapted from MCNPX. This will be extended to work directly with the existing mesh-based weight windows on the same mesh;
- K-effective source correlation correction: This involves analysis of the correlation of source points between cycles to improve the confidence interval in criticality calculations;
- Completion of the pulse-height tally/variance reduction enhancements for electron and coupled P/E modes;
- Extend the period of the random number generator;
- Further work on modularization;
- Further enhancements to parallelism: Use of collective operations has been shown to dramatically increase the parallel scalability and efficiency.

We are also funding R. Schwarz and L. L. Carter to update the MCNP Visual Editor[16] (VISED) to MCNP V5 to provide a path to improved user-setup capabilities.

Conclusions

A tremendous amount of work has been done (and continues to be done) on MCNP to prepare for the release of MCNP Version 5. The work to modernize this code has required modification of every single line of code and the work will continue as MCNP evolves in the future.

We look forward to continuing our support of our international user-base. We will strive to ease the transition to the new code by a continuing commitment to user support and training.

Acknowledgements

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