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MCNP Monte Carlo Progress – Nuclear Criticality Safety

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INTRODUCTION

MCNP is a mature, robust, continuous-energy Monte Carlo code. It has been used to perform high-fidelity benchmark calculations for cross-sections, calculations for critical experiment design, analyses for criticality safety problems, and very many other applications since the 1970s. For the past 10 years, the production release of the code has been MCNP5 [1], with over 10,000 copies distributed throughout the world [2]. The next major version of the code, MCNP6 [3], is in beta testing and nearing completion. This paper summarizes progress during FY 2012 in the development and support of MCNP for the US DOE Nuclear Criticality Safety Program. Activities and accomplishments are summarized in five major areas:

- MCNP5 and MCNP6 status,
- Verification and validation testing,
- User support & training,
- Work in progress, and
- Future release plans.

MCNP5 AND MCNP6 STATUS

The latest production release of the MCNP5 Monte Carlo code is designated MCNP5-1.60 [4-6]. This version was developed during 2009-2010 and included in RSICC releases in October 2010, July 2011, and February 2012. The focus for this release was to provide end-users with stability and reliability for criticality calculations, support for the latest computers, and rigorous and extensive code verification/validation.

MCNP5-1.60 includes enhancements to several MCNP capabilities: maximum number of cells, surfaces, materials, and tallies; isotopic reaction rates for mesh tallies; and adjoint-weighting for computing effective lifetimes and delayed neutron parameters.

The MCNP6 Monte Carlo code has been under development since 2004, when a version of MCNP5 was modified to include capabilities for modeling high-energy protons and used locally for analyzing proton radiography experiments. Over the past 4 years, many additional capabilities for high-energy physics, depletion, and detector modeling have been merged from the MCNPX [7] Monte Carlo code into MCNP6. MCNP6 can currently model 36 different particle types as well as heavy ions. MCNP6 includes all features and capabilities found in MCNP5 and MCNPX, plus additional recently developed capabilities. Figure 1 illustrates the relationships among the versions of MCNP. It should be noted that all future Monte Carlo development at LANL is focused on MCNP6.

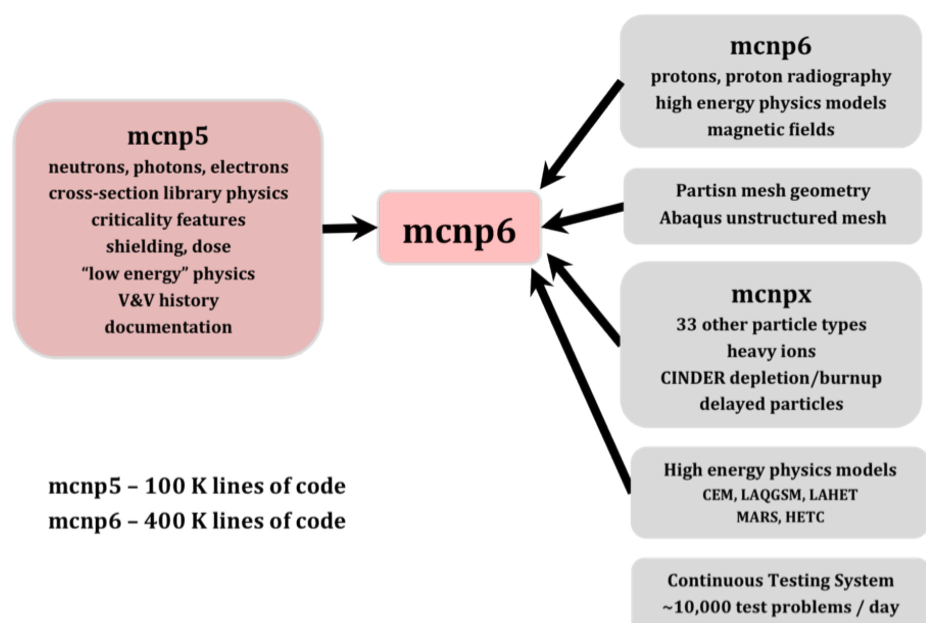

Fig. 1. Relationships Among Versions of MCNP

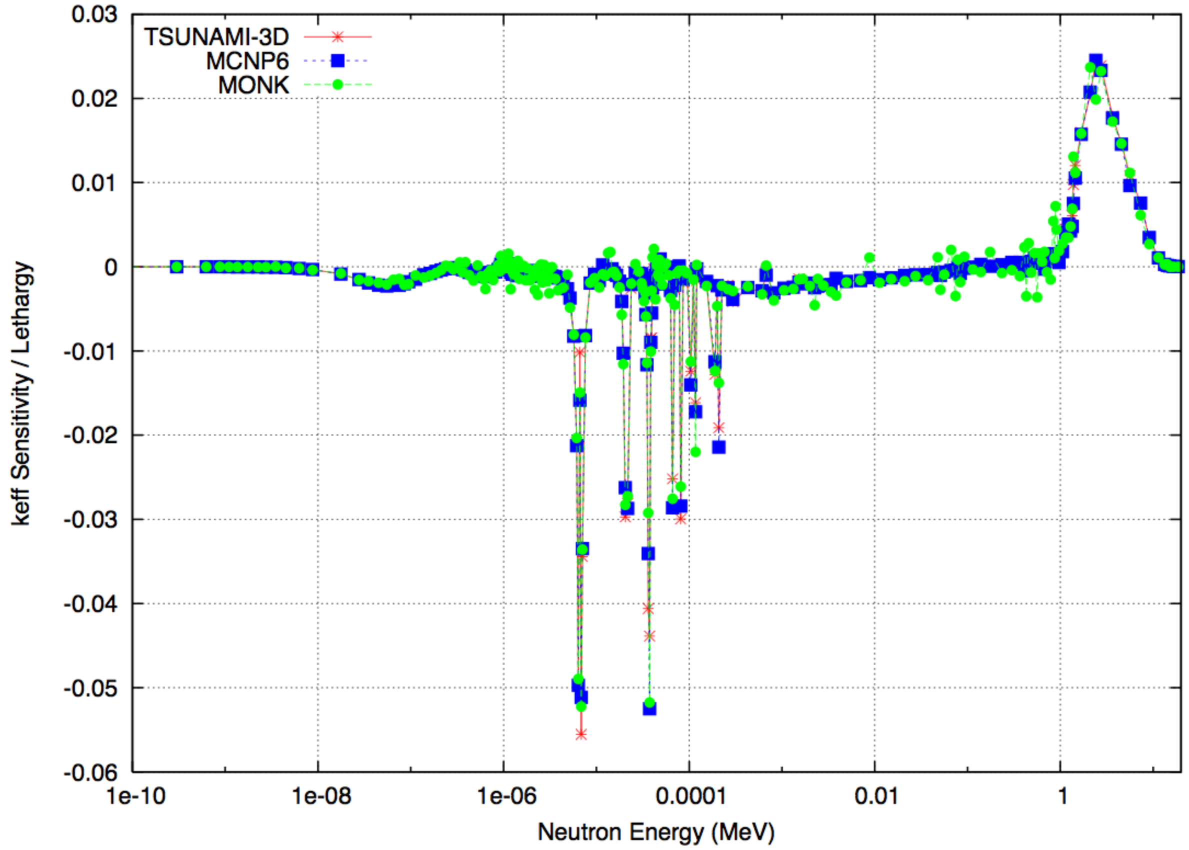

Fig. 2. ^{238}U total cross-section sensitivity for a water-moderated MOX fuel assembly. Continuous-energy results for MCNP6 and MONK, Multigroup results for TSUNAMI-3D.

MCNP6 includes all of the features found in MCNP5-1.60 for criticality safety support, along with new capabilities for continuous-energy adjoint-weighted perturbation analysis [8]; continuous-energy sensitivity-uncertainty analysis of neutron cross-section data [9] (see Fig. 2 for an example); use of a fission matrix to estimate the eigenvalue, dominance ratio, and eigenfunction; and the initial implementation of On-The-Fly Doppler broadening of neutron cross-sections [10]. Many other new features in MCNP6, such as proton radiography and embedded mesh geometry illustrated in Fig. 3, are less important at present to criticality safety applications, but may be important for a variety of future uses.

Both MCNP5 and MCNP6 were used extensively in testing performed for the evaluation and release of the ENDF/B-VII.1 nuclear data libraries [11].

VERIFICATION AND VALIDATION TESTING

Throughout the 35+ year history of MCNP, ongoing, serious effort has been devoted to ensuring that MCNP provides reliable, accurate results for criticality safety applications with the best available cross-section data. The MCNP website (mcnp.lanl.gov) provides over 50 verification/validation reports for criticality safety and cross-section data evaluation, and current MCNP code distributions from RSICC include hundreds of ICSBEP [12] problems used in the routine evaluation of MCNP. A recent report [13,14] documents the testing of both MCNP5-1.60 and MCNP6-Beta-2 in early 2012 for use in criticality safety calculations. That work emphatically documents the fact that MCNP6-Beta-2 reproduces all results from MCNP5-1.60, when both codes are compiled with the same Fortran-90 compiler and options. Verifying that the new code, MCNP6-Beta-2, matches results with the proven production version, MCNP5-1.60, is important for both verifying MCNP6 and for easing the eventual migration of users from MCNP5 to MCNP6. See [14] at this meeting for further details.

In addition to the detailed verification efforts using hundreds of ICSBEP problems, MCNP6 undergoes continuous, 24/7 testing using an automated test system. A smaller set of 31 ICSBEP problems and a set of 10 problems from the analytical criticality benchmark suite are run each night. This automated testing ensures that changes to the MCNP6 code base do not affect the results of criticality benchmark problems.

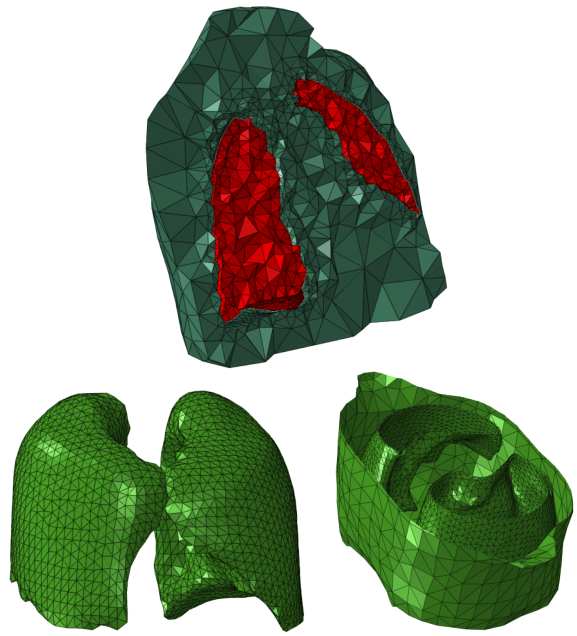

Fig. 3. Example of 3D unstructured mesh geometry for MCNP6, human torso and lungs (courtesy Prof. G. Xu, RPI)

USER SUPPORT & TRAINING

The MCNP development team continues to provide a high level of user support, including 3-4 1-week introductory classes on MCNP each year at LANL; several on-site classes at other Laboratories targeted toward criticality safety specialists; a new, completely updated website; a reference collection of over 550 documents (1 GB in size) of PDF reports and papers on all aspects of MCNP – theory, practice, V&V, parallel computing, etc.; and the 1,000-member MCNP Forum email group. We also help to assist users in the installation and use of MCNP on a large number of different computer platforms – Windows, Macs, Linux, Unix, threaded parallelism on laptops and desktops, MPI parallel use on clusters, various Fortran compilers, etc.

WORK IN PROGRESS

Given the age of MCNP (35+ years is an eternity for computer software), the large number of features, the large size of the code, and the wide variety of computer platforms supported, maintenance of the existing code is easily a full-time job for several people. Nevertheless, we devote significant effort to Monte Carlo research and development (R&D), publish roughly 50 technical documents per year, and are committed to advancing the state-of-the-art for Monte Carlo calculations. Part of the continued success of this ongoing R&D effort is due to collaboration with several universities, leveraging the creativity of talented graduate students with the expertise of the MCNP development team.

The new features described above for MCNP5 and MCNP6 are examples of R&D work from the 2011-12 timeframe that were successful and are about to be released. Examples of current R&D work (of which some may work and some may not) include:

- Use of the fission matrix for accelerating the convergence of Monte Carlo criticality calculations
- Investigation of higher eigenvalues and eigenmodes for alpha-eigenvalue calculations
- New iteration strategies for both k- and alpha-eigenvalue calculations
- New schemes to eliminate the under-estimation of confidence intervals for local reaction rates and power in criticality calculations
- The use of a spatially continuous Monte Carlo estimator to evaluate whether neutron histories provide adequate coverage of the problem phase space
- Improved resonance scattering treatments in the epithermal neutron energy range
- Novel approaches to exascale-parallelism for Monte Carlo particle transport, including data decomposition
- Restructuring portions of MCNP6 in a more object-oriented, developer-friendly manner
- Improvements to the capabilities for reactor depletion calculations, especially in lowering the memory footprint to enable larger problem sizes
- Continuous-energy capabilities for uncertainty quantification
- Interface sensitivities for geometric tolerances
- Enhanced mesh tallies, providing partial currents for each surface of a mesh cell

FUTURE RELEASE PLANS

Future releases of MCNP are focused on MCNP6, especially since we have verified that it will match criticality results obtained with MCNP5-1.60. Precise dates for a production-level release of MCNP6 should not be simply legislated by funding, management, or wishful thinking; there is still serious work required to update the MCNP6 documentation, extend the verification/validation basis in several areas, clean up and better organize some of the coding after the recent large expansion of the MCNP code base, and provide guidance to users in migrating from older versions to MCNP6. Given the enormous investment over the past 35+ years in developing MCNP, much care must be taken to ensure that an upgrade to MCNP6 produces a reliable, trustworthy, documented, verified product that fully meets the needs of the user community. A number of the MCNP developers are working diligently to ensure a successful release of MCNP6, and to build user confidence in and support for MCNP6. We are targeting another beta release of MCNP6 during the Fall/Winter of 2012, and a production release during 2013.

REFERENCES

1. X-5 MONTE CARLO TEAM, “MCNP – A General N-Particle Transport Code, Version 5 – Volume I: Overview and Theory”, LA-UR-03-1987, Los Alamos National Laboratory (April, 2003).
2. RSICC, personal communication (2011).
3. MCNP6 DEVELOPMENT TEAM, "Initial MCNP6 Release Overview - MCNP6 Beta 2", LA-UR-11-07082 (2011).
4. F.B. BROWN, B.C. KIEDROWSKI, J.S. BULL, "MCNP5-1.60 Release Notes", LA-UR-10-06235, Los Alamos National Laboratory (2010).
5. B.C. KIEDROWSKI, ET AL., "MCNP5-1.60 Feature Enhancements & Manual Clarifications", LA-UR-10-06217, Los Alamos National Laboratory (2010).
6. F.B. BROWN, B.C. KIEDROWSKI, J.S. BULL, M. GONZALES, N. GIBSON, "Verification of MCNP5-1.60", LA-UR-10-05611, Los Alamos National Laboratory (2010).
7. DENISE B. PELOWITZ, ET AL., "MCNPX 2.7.0 Extensions", LA-UR-11-02295, Los Alamos National Laboratory (2011).
8. B.C. KIEDROWSKI, F.B. BROWN, “Comparison Of The Monte Carlo Adjoint-Weighted And Differential Operator Perturbation Methods”, *Proceedings SNA+MC-2010*, Tokyo, Oct 17-20 (2010).
9. B.C. KIEDROWSKI, F.B. BROWN, “Continuous-Energy Sensitivity Coefficient Capability in MCNP6”, *Trans. Am. Nuc. Soc.* **107** (2012).
10. F.B. BROWN, W.R. MARTIN, G. YESILYURT, S. WILDERMAN, "Progress with On-The-Fly Neutron Doppler Broadening in MCNP", *Trans. Am. Nuc. Soc.* **106** (2012).
11. OECD NUCLEAR ENERGY AGENCY, *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, NEA/NSC/DOC(95)03, (2007).
12. A.C. KAHLER, ET. AL., “ENDF/B-VII.1 Neutron Cross Section Data Testing with Critical Assembly Benchmarks and Reactor Experiments”, *Nuclear Data Sheets*, Vol. 112, No. 12 (2011).
13. F.B. BROWN, B.C. KIEDROWSKI, J.S. BULL, "Verification of MCNP5-1.60 and MCNP6-Beta-2 for Criticality Safety Applications", LA-UR-12-21041, Los Alamos National Laboratory (2012).
14. B.C. KIEDROWSKI, F.B. BROWN, J.S. BULL, "Verification of MCNP5-1.60 and MCNP6-Beta-2 for Criticality Safety Applications", *Trans. Am. Nuc. Soc*. **107** (2012)