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MCNP Developments

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INTRODUCTION

The MCNP Monte Carlo code has been used for high-fidelity analyses of criticality safety problems since the 1970s. This paper summarizes progress during FY 2010 and early FY 2011 in the development and support of the MCNP code under the US DOE Nuclear Criticality Safety Program. Activities and accomplishments are summarized in five major areas:

- MCNP5-1.60 release,
- Verification and validation testing,
- User support & training,
- Work in progress, and
- Future release plans.

MCNP5-1.60 RELEASE

The latest release of the MCNP5 [1-3] Monte Carlo code is designated MCNP5-1.60 [4-6]. This version was developed during Fall 2009 – Spring 2010, tested extensively during Summer 2010, and then sent to RSICC for release in September/October 2010. The focus for this release was to provide end-users with: (1) stability and reliability for criticality calculations, (2) support for the latest computers, including multicore CPUs, Windows-Mac-Linux platforms, and 32/64 bit systems, (3) rigorous and extensive code verification/validation, and (4) a few new features and a number of minor bug-fixes. All previously existing code capabilities are preserved, including physics options, geometry, tallying, plotting, cross-section handling, etc. No errors were found that would affect the code results for basic criticality calculations.

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.

Extensive verification and validation testing was performed, involving roughly 5,000 hrs of computing time. Tally results from MCNP5-1.60 are expected to match the tally results of problems that can be run with the previous MCNP5-1.51 [2,3], except where bugs were discovered and fixed. The bug fixes and enhancements are discussed in [4], supplemental pages for the MCNP manual are provided in [5], and verification/validation work is described in [6]. In the sections below, we

summarize the code enhancements and provide some results from the verification/validation effort.

New Features

Adjoint-weighted tallies for point kinetics

parameters: For the first time, MCNP5-1.60 includes the capability to generate adjoint-weighted reactor kinetics parameters from continuous-energy Monte Carlo. The adjoint response function used for criticality calculations is the iterated fission probability. The neutron generation time Λ and the effective delayed neutron fraction β_{eff} are expressed as ratios of adjoint-weighted integrals.

Mesh tallies for isotopic reaction rates: With MCNP5-1.60, use of the FM cards for mesh tallies has been extended to handle isotopic mesh tallies as well, so that users do not need to enter number densities directly for isotopic mesh tallies; the mesh tally routines can now find the actual problem materials and use the appropriate number densities in performing the isotopic reaction rate tallies.

Increased limits for geometry, tally, and source specifications: MCNP5-1.60 includes modifications that extend the limits on the number of cells, surfaces, materials, etc., from a maximum of 99,999 to 99,999,999. The maximum number of tally card identifiers is also raised from 999 to 9,999. Detailed discussion of these changes is found in [5].

Web-based documentation: The documentation for MCNP5-1.60 includes over 300 MB of reference material organized in an easy to access, web-based format that can be viewed in any web browser.

Utility programs: The *merge_mctal* and *merge_meshtal* utilities are used to merge separate *mctal* or *meshtal* files, respectively, from different independent MCNP5 jobs. Both were updated and made more general.

General improvements: The general enhancements include: build system improvements, random number generator options, number of nesting levels for universes, support for threading on multicore computers, parallel processing efficiency improvements for threaded criticality calculations, arbitrary number of threads for restart (continue) runs, 12 other minor enhancements to the code, and 30 minor bug-fixes, none of which affect results for criticality calculations.

Verification / Validation

To verify that the MCNP5-1.60 is performing correctly, several suites of verification/validation problems were run. Results have been compared with previously verified versions of MCNP5, with experimental or analytic results, and with results from running on different computer hardware/software platforms. In addition, two new verification/validation suites have been added, the Kobayashi benchmarks with problems containing voids and ducts, and a set of benchmarks for reactor kinetics parameters. The testing suites are:

Regression - The standard MCNP5 Regression Test Suite [1,3] used for code development and installation testing was expanded from 52 to 66 problems.

VALIDATION_CRITICALITY [9] - 31 problems from the *International Handbook of Evaluated Criticality Benchmark Experiments* [10], modified to permit running with either ENDF/B-VI data libraries or the newer ENDF/B-VII.0 data libraries.

VERIFICATION_KEFF - 75 criticality problems found in the literature for which exact analytical solutions are known [11].

VALIDATION_SHIELDING - 19 shielding and dose calculations [9,12], including time-of-flight spectra for neutrons from pulsed spheres, neutron and photon spectra at shield walls within a simulated fusion reactor, and photon dose rates. This suite was overhauled to compare plots of results against experimental data.

KOBAYASHI - The “Kobayashi Benchmarks” [13] were added. These benchmark problems consist of simple 3D geometries that contain at least one void region and one mono-energetic, isotropic, cubic source region. Each is simulated first with a purely absorbing and then with a fifty-percent scattering medium, with fluxes calculated using point detector tallies. Overall, 136 different fluxes were compared between computed MCNP5 results and the reference results.

POINT_KINETICS - A series of problems was added to test the new ability to compute reactor kinetics parameters [7,8]: neutron generation times, Rossi- α , total and precursor-specific effective delayed neutron fractions, and average precursor decay constants. The verification problems are compared against both analytic solutions and discrete ordinates results from Partisn [14]. For validation, six values of Rossi-alpha are compared to experimentally measured values from the ICSBEP handbook [10].

Summary of testing: Verification calculations for MCNP5-1.60 were run on Mac OS X, Linux, and Windows computing systems using 1 CPU, threading on multicore CPUs, parallel MPI message-passing, and mixed MPI+threading, and several different Fortran-90 compilers on each computer platform. The total computing time for testing was approximately 5,000

CPU-hours. Results from these calculations have been compared to results from the previous, verified version of MCNP5 (Version 1.51), to known analytical results, and to results from experiments.

Based on the excellent agreement found in all cases run, we conclude that all of the previous verification/validation efforts carried out in support of MCNP should carry over to the present version, MCNP5-1.60. We do not presume to declare MCNP5-1.60 as validated for any particular end-user application (that is the prerogative of the end-users, for their specific requirements and applications of the code), but suggest that such validation should be straightforward given the results obtained for the MCNP5-1.60 verification testing. MCNP5-1.60 can be obtained from RSICC (rsicc.ornl.gov).

VERIFICATION AND VALIDATION TESTING

Significant effort has been focused on extending the suites of problems used for verification/validation testing of MCNP. The goals are to move toward physics-based comparisons against experiment or exact analytic results; to include the verification/validation suites in the MCNP permanent code repository and RSICC distributions; to automate the testing for easy execution; and to automate the collection of results and comparison to experiment. For validation of the new features for computing Rossi- α , β_{eff} , and Λ_{eff} , the Rossi Alpha Validation Suite [15] was developed. It includes 12 ICSBEP benchmarks – 4 HEU, 3 IEU, 3 Pu, and 2 ^{233}U – of which 8 are fast, 2 intermediate, and 2 thermal spectra. In addition, the new Expanded Criticality Validation Suite [16] includes 119 ICSBEP benchmark problems covering a broad range of fissile material, geometries, and spectra.

USER SUPPORT & TRAINING

We have continued to provide extensive support to MCNP end-users for criticality safety calculations. During the past year 3 criticality classes were given at DOE sites, and 4 general classes were given at LANL. A half-day workshop on advanced Monte Carlo methods was presented at the PHYSOR-2010 conference, and more than 10 papers and associated talks were given at international conferences.

To provide a means for users and code developers to interchange ideas and advice, provide feedback, and report bugs, the MCNP Forum email list forum continues, with about 1,000 members world-wide.

Over the past 50 years there has been extensive documentation of Monte Carlo methods and the MCNP code, but much of the literature is difficult to find today. To make this extensive literature readily available, the MCNP Reference Collection has been assembled, with browser-based access to over 500 technical reports

comprising over 1 GB of PDF files. This collection will be distributed with future MCNP releases.

We have continued to maintain close collaboration with a number of universities, including the University of Michigan, the University of New Mexico, the University of Wisconsin, Oregon State University, MIT, and RPI.

WORK IN PROGRESS

Most of the development in MCNP5 in 2010 has been devoted to nuclear criticality safety. Adjoint-weighted tallies have been developed with the primary application of computing sensitivity coefficients using continuous-energy physics. The issue of statistical coverage has also been investigated.

Adjoint-Weighted Tallies for Sensitivity Analysis

Proper design of integral experiments requires the calculation of sensitivity coefficients for nuclear cross sections to ensure that the experiment provides useful information. The SCALE package computes sensitivity coefficients with multigroup cross section data using the TSUNAMI package and adjoint-based perturbation theory. The MCNP approach uses the same adjoint-based methodology except that the calculations are done inline and with continuous-energy physics.

Work over the last three years has produced the routines for inline adjoint-weighted tallies based upon the idea of the iterated fission probability. These have been successfully applied to using continuous-energy Monte Carlo to estimate point kinetics parameters and have been extended to performing adjoint-based perturbation theory [7].

Similar methodologies are employed to compute sensitivity coefficients. Verification has been performed in multigroup and by comparing with results generated by TSUNAMI for continuous energy [17]. It was found that the multigroup results show excellent agreement along with continuous-energy variants for capture and fission sensitivities. Scattering still needs to be addressed and work is underway to incorporate the probability densities of the scattering laws.

Recent investigations have also focused on the computation of sensitivity to system dimensions. This is useful to understand which interface locations are important and to decide tolerance specifications. A prototype has been prepared that appears to show promising results [17].

Statistical Coverage and Population Diagnostics

A fundamental issue with eigenvalue calculations in Monte Carlo is convergence to the fundamental mode because the steady-state source is unknown a priori. Many

applications in criticality safety involve discrete zones of fissile material that are particularly problematic.

Over the last several years, much analysis has been done on the issue of source convergence. Implicit in this analysis is the assumption that the population sizes are large enough such that all regions have a sufficiently high population.

A modified version of the “K-effective of the World” problem has been created to simulate a flooded subcritical assembly storage vault [19]. This problem is a $9 \times 9 \times 9$ array of subcritical Pu-239 spheres ($k = 0.95$) with the central sphere exactly critical when immersed in water. The central sphere is also isolated with a thick cadmium coating such that the coupling is asymmetric: it is far easier for neutrons to communicate with the other spheres than those to communicate with it. Even applying the best practices using batch sizes of 5K, 10K, and 20K neutrons, it is shown that there is a non-trivial probability of achieving the wrong answer because the central sphere is inadequately sampled.

This test problem demonstrates potential dangers that a criticality safety practitioner may face in particular situations. This motivates future research for the development of robust population diagnostics.

FUTURE RELEASE PLANS

The MCNP6 Monte Carlo code constitutes a merger of the MCNP5 and MCNPX [20] codes, and has been under development for the past few years. It includes many additional capabilities for high-energy physics, depletion, and detector modeling from MCNPX. MCNP6 can currently model 36 different particle types as well as heavy ions. Additionally, many new MCNP features have been developed for MCNP6, including adjoint-weighted tallies for perturbations and sensitivity/uncertainty applications. MCNP6 thus includes all features and capabilities found in MCNP5 and MCNPX, plus additional recently developed capabilities. Many additional verification/validation suites have been developed to cover the new ranges of analysis and capabilities. Limited beta testing of MCNP6 outside of LANL began in early 2011. A more general beta test period is planned for the Fall of 2011, and then a fully supported production release in 2012. It is expected that all subsequent development and support will be focused on MCNP6, the unified and extended code. End-users in all application areas need to be aware of the forthcoming MCNP6 release and begin planning for the transition to the new code in 2012 and beyond.

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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. F.B. BROWN, J.S. BULL, J.T. GOORLEY, A. SOOD, J.E. SWEEZY, "MCNP5-1.51 Release Notes", LA-UR-09-00384, Los Alamos National Laboratory (2009).
3. F.B. BROWN, J.E. SWEEZY, J.S. BULL, A. SOOD, "Verification of MCNP5-1.50", LA-UR-08-3443, Los Alamos National Laboratory (2008).
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. B.C. KIEDROWSKI, F.B. BROWN, P. WILSON, "Calculating Kinetics Parameters and Reactivity Changes with Continuous Energy Monte Carlo", *Proc. PHYSOR-2010*, Pittsburgh, PA (2010).
8. B.C. KIEDROWSKI, "Theory, Interface, Verification, Validation, and Performance of the Adjoint-Weighted Point Reactor Kinetics Parameter Calculations in MCNP", LA-UR-10-01700, Los Alamos National Laboratory (2010).
9. R.D. MOSTELLER, "Validation Suites for MCNP," *Proc. of the American Nuclear Society Radiation Protection and Shielding Division 12th Biennial Topical Meeting*, Santa Fe, New Mexico (April 2002).
10. International Handbook of Evaluated Criticality Safety Benchmark Experiments, NEA/NSC/DOC(95)03, OECD Nuclear Energy Agency (2008).
11. A. SOOD, R. A. FORSTER, AND D.K. PARSONS, "Analytical Benchmark Test Set for Criticality Code Verification," *Prog. Nucl. Energy*, 42, pp. 55-106 (2003).
12. J. A. BUCHOLZ & S. C. FRANKLE, "Improving the LLNL Pulsed Sphere Experiments Database and MCNP Models", *Trans. Am. Nucl. Soc.* (2003).
13. K. KOBAYASHI, N. SUGIMURI, Y. NAGAYA, "3-D Radiation Transport Benchmark Problems and Results for Simple Geometries with Void Regions", OECD/NEA Report (Nov., 2000)
14. R.E. ALCOUFFE, et al. "Partisn Manual", LA-UR-02-5633, Los Alamos National Laboratory (2002).
15. R.D. MOSTELLER & B.C. KIEDROWSKI, "A Rossi Alpha Validation Suite for MCNP", ICNC-2011, Edinburgh Scotland [also LA-UR-11-01162] (2011).
16. R.D. MOSTELLER, "An Expanded Criticality Validation Suite for MCNP", LA-UR-10-06230 (2010).
17. B.C. KIEDROWSKI, J.A. FAVORITE, F.B. BROWN, "Verification of the k-Eigenvalue Sensitivity Coefficient Calculations Using Adjoint-Weighted Perturbation Theory in MCNP", *Trans. Am. Nucl. Soc.* (2010).
18. B.C. KIEDROWSKI, J.A. FAVORITE, F.B. BROWN, "Monte Carlo Calculations of Eigenvalue Sensitivities to System Dimensions," LA-UR-11-01321, Los Alamos National Laboratory (2011).
19. B.C. KIEDROWSKI, F.B. BROWN, "Statistical Coverage Concerns in a Revised k-Effective of the World Problem" LA-UR-11-00046, Los Alamos National Laboratory (2011).
20. M.R. JAMES, et al., "MCNPX 2.7.X - New Features Being Developed," LA-UR-09-6788, IEEE/NSS Conference, Orlando, FL, October 25-31 (2009).