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MCNP6 Shielding Validation Suite: Past, Present, and Future

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INTRODUCTION

Extensive validation of MCNP5/6 [1,2] has been performed over the last several years for criticality benchmarks [3,4]. The MCNP development team continually improves the validation capabilities in this area [5].

Far less attention, however, has been given to the MCNP shielding benchmark suite [3]. This is despite the fact that MCNP is often used for criticality accident assessment and alarm design, an application of direct importance to the U.S. Department of Energy Nuclear Criticality Safety Program.

Recent work improved these shielding benchmarks and new validation calculations were performed [3]. Like with the criticality suite, automation of running and data processing is implemented. Plans for new benchmarks, including those in Volume VIII of the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP) [6] for inclusion into the MCNP6 Shielding Validation Suite are discussed.

Status of the "Legacy Suite"

The MCNP5 Shielding Suite had a series of input files from various programs: LLNL pulsed spheres [7], fusion shielding [8], and photon dose benchmarks [9,10]. Table I contains information on the benchmarks in what will from now on be termed the "Legacy Suite".

Unfortunately, the results obtained for the corresponding MCNP inputs are very limited, and validation was performed very infrequently by the MCNP team. Unlike with the criticality benchmarks, the Suite did not compare to experimental results, but only served as a sporadically used regression tool.

EVOLUTION OF THE SUITE

The goal of improving the suite is done in three phases. First is the identification of experimental results, their placement within the MCNP distribution, and, if necessary, modification of the existing input files for better comparison with

Table I: Contents of the Legacy Suite

| Туре | Material/Description | | |
|---------------|---|--|--|
| Pulsed Sphere | Lithium-6 | | |
| | Beryllium | | |
| | Carbon | | |
| | Nitrogen | | |
| | Iron | | |
| | Lead | | |
| | Water | | |
| | Concrete | | |
| Fusion | Config. 1, Neutron, On-Axis | | |
| Shielding | Config. 3, Neutron, Off-Axis | | |
| | Config. 3, Photon, On-Axis | | |
| | Config. 7, Neutron, On-Axis | | |
| | Config. 7, Photon, Off-Axis | | |
| Photon Dose | Co-60 Skyshine | | |
| | Co-60 Air Over Ground | | |
| | Co-60 Through Air | | |
| | Co-60 Through Teflon | | |
| | Sm K_{α} Through Air | | |
| | $\operatorname{Sm} K_{\alpha}$ Through Teflon | | |

experiment. The second phase involves automating the test suite so that the problems are run, producing plots in .pdf format, and offering condensed metrics for comparison of nuclear cross section datasets. The third phase involves the identification of new problems to provide greater coverage for the suite.

Comparisons with Experiment

For the existing problems in the suite, experimental data was lifted from reports [7-9] and placed alongside the MCNP input files. Unfortunately, no experimental data was found for the photon dose benchmarks other than the skyshine experiment and these were consequently removed from the suite. Since these are permanently stored within the MCNP development archive, should experimental data by found, these can easily be restored.

For the LLNL pulsed spheres, the old MCNP inputs only provided three time intervals over which tallies were made. The tally specifications of these

have been modified to match the time-binning structure of the experimental results. This was likewise done for the fusion shielding benchmarks as well. The MCNP input files for the skyshine experiments did not require modification other than to combine several tallies into one for convenience in plotting.

With new MCNP input files, calculations were run with ENDF/B-VII.0 nuclear data and comparisons with experiment were made. MCNP6 can generally reproduce the experimental results with some notable exceptions such as the fusion neutron peaks of the benchmarks.

Automation

For MCNP developers and users, it should be simple to run the validation suite, and have results generated in convenient formats. For the development team, this serves as a convenient means to perform software regression and assist nuclear data efforts with testing of new cross section sets, such as ENDF/B-VII.1. For users performing shielding calculations, these benchmarks can serve as a means of starting validation for their specific applications.

Like the criticality validation suites, a Makefile is provided to run the problem and produce conveniently readable outputs. For criticality problems, this is typically one result: k_{eff} ; however, for shielding, often numerous data points, such as those for a spectrum, are obtained.

For this reason, both the calculated MCNP and experimental results are provided in the "mctal" file format. These files are read by the MCNP plotter and



Fig. 1. Comparison of MCNP calculation to experiment for the carbon sphere. MCNP is solid black and experiment is dashed blue.

| Material | Average | 90-Percentile |
|----------|---------|---------------|
| Li-6 | 0.183 | 0.356 |
| Be | 0.114 | 0.224 |
| С | 0.150 | 0.247 |
| Ν | 0.134 | 0.246 |
| Fe | 0.155 | 0.280 |
| Pb | 0.122 | 0.221 |
| Water | 0.292 | 0.610 |
| Concrete | 0.129 | 0.235 |

a postscript file is generated to provide developers and users with results that can be visualized. An example of results from the carbon LLNL pulsed sphere is given in Fig. 1.

For the LLNL pulsed spheres and the fusion shielding benchmarks, aggregate results for each benchmark are calculated in two different ways: First is the average relative error (with respect to the experimental result), and second is the 90th percentile of the same result. Since issues with resolving the peaks are known with the LLNL pulsed spheres, and may be related to specifications, the first ten time bins are excluded from these aggregate error metrics. Table II provides these aggregates for the LLNL pulsed spheres using ENDF/B-VII.0.

Future Additions

With the removal of some benchmarks, the number in the Suite now stands at 14. As such, the coverage for this suite is quite limited.

Additional LLNL pulsed sphere benchmarks featuring different materials are available, but not included. These include: Li-7. O, Mg, Al, Ti, Heavy Water, Polyethylene, Teflon, U-235, U-238, and Pu-239. This would bring the suite up to 25 benchmarks, and increase the coverage of materials.

Volume VIII of the 2010 edition of the ICSBEP features six "criticality alarm" benchmarks. Three of these are shielding problems involving a Cf-252 source surrounded by air and spheres of iron and lead. While these two materials are also included in the LLNL pulsed spheres, the spontaneous fission spectrum tests qualitatively different (albeit overlapping) physics regimes.

Two benchmarks are provided of the "labyrinth" type featuring a concrete duct streaming-type arrangement. The configurations use the same geometry, but one involves a bare Cf-252 source and another shielded by a polyethylene sphere. The remaining benchmark is another skyshine experiment.

In addition to those contained within the ICSBEP, a duct streaming problem evaluating the albedo of neutrons on concrete in one-, two-, and three-legged duct configurations appears to be a promising candidate [11].

SUMMARY

With the upcoming release of MCNP6 and its new capabilities, it is likewise important to improve the validation for core features, especially considering that these are directly relevant to areas of the criticality safety community.

The Legacy Suite was a list of benchmarks that did not offer any convenient means to compare MCNP results with experimental data and only served as a regression suite. Improvements have been made that facilitate its role as a validation suite much in the same way as the current criticality validation suites do currently. For example, the experimental data is stored in a convenient format such that the MCNP plotter can automatically generate plots for visual comparisons of calculation to experiment.

New additions to the MCNP6 Shielding Validation Suite are currently being investigated and several candidates have been identified from the LLNL pulsed sphere program, the ICSBEP, and a neutron albedo/duct streaming benchmark.

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REFERENCES

- 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 (2003).
- 2. J.T. GOORLEY, et. al., "Initial MCNP6 Release Overview," LA-UR-11-01766, Los Alamos National Laboratory (2011).
- F.B. BROWN, et. al., "Validation of MCNP5-1.60", LA-UR-10-05611, Los Alamos National Laboratory (2010).
- 4. R.D. MOSTELLER, "Validation Suites for MCNP", Proc. ANS Radiation Protection and Shielding Division 12th Biennial Topical Meeting, Santa Fe, New Mexico (2002).

- R.D. MOSTELLER, "An Expanded Criticality Validation Suite for MCNP," LA-UR-10-06230, Los Alamos National Laboratory (2011).
- 6. J.B. BRIGGS (Ed.), "International Handbook of Evaluated Criticality Safety Benchmark Experiments," Nuclear Energy Agency, Paris, France (2010).
- C. WONG, et. al., "Livermore Pulsed Sphere Program: Program Summary through July 1971," UCRL-51144 Rev. I, Lawrence Livermore National Laboratory (1972).
- P.F. ROSE, R.W. ROUSSIN (Eds.), "Shielding Benchmark Compilation," BNL-19302, Vol. 2, Brookhaven National Laboratory (1983).
- R.R. NASON, J.K. SHULTIS, R.E. FAW, "A Benchmark Gamma-Ray Skyshine Experiment," *Nucl. Sci. & Eng.*, 79, p. 404-416 (1981).
- D.J. WHALEN, D.E HOLLOWELL, J.S. HENDRICKS, "MCNP: Photon Benchmark Problems," LA-12196, Los Alamos National Laboratory (1991).
- 11. C.J. SOLOMON, A. SOOD, "Duct Streaming Validation Benchmark Calculations with a Global Importance Map," *Trans. Am. Nucl. Soc.*, **101**, p. 638-642 (2009).