LA-UR-17-20668

Title: Semi-Analytical Benchmarks for MCNP6

Author(s): Grechanuk, Pavel
Rising, Michael Evan
Brown, Forrest B.
Palmer, Todd S.

Intended for: 2017 American Nuclear Society Annual Meeting, 2017-06-11/2017-06-15
(San Francisco, California, United States)

Issued: 2017-04-03 (rev.1)

Semi-Analytical Benchmarks for MCNP6

Pavel Grechanuk[1] Michael E. Rising[2], Forrest B. Brown[2], and Todd S. Palmer[1]

[1] *Nuclear Engineering and Radiation Health Physics Department, Oregon State University, Corvallis, OR, 97331, USA*
[2] *XCP-3 Computational Physics Group, Los Alamos National Laboratory, MS B283, Los Alamos, NM 87545, USA*
grechanp@oregonstate.edu, mrising@lanl.gov, fbrown@lanl.gov, palmerts@engr.orst.edu

INTRODUCTION

Code verification is an extremely important process that involves proving or disproving the validity of code algorithms by comparing them against analytical results of the underlying physics or mathematical theory on which the code is based upon. Monte Carlo transport codes such as MCNP6 [1, 2] undergo verification and testing upon every release to ensure that the codes are properly simulating nature. Specifically, MCNP6 has multiple sets of problems with known analytic solutions that are used for code verification [3, 4].

Most of the verification problems are fairly simple due to the fact that they are usually composed of few materials, with simplified cross-sections, or physics approximations, and simple geometry. These approximations make the transport equation possible to solve analytically or semi-analytically, and thus they are quite valuable in verifying that the code algorithms and methods (Monte Carlo, discrete ordinates, etc.) are operating as intended. The remainder of this paper is organized as follows: first we briefly discuss the theory behind the benchmarks problems, then the numerical results are presented, and finally we conclude with general remarks on this and possible future work.

THEORY

Most of the analytical benchmarks for fixed source transport problems used for code verification specify either the boundary conditions for the angular or scalar flux or the external (usually isotropic) source. Monte Carlo codes on the other hand, primarily specify either current boundary sources or a volumetric fixed source, either of which can be very complicated functions of space, energy, direction and time. Thus, most of the challenges with modeling analytic benchmark problems in Monte Carlo codes come from identifying the correct source definition to properly simulate the correct boundary conditions [5]. In this benchmark suite, the problems included originate from chapter 3 of Professor Barry Ganapol's book, *Analytical Benchmarks for Nuclear Engineering Applications Case Studies in Neutron Transport Theory* [6].

The class of problems included in this suite all deal with mono-energetic neutron transport without energy loss, in a homogeneous material. The variables that differ between the problems are source type (isotropic/beam), medium dimensionality (infinite/semi-infinite/finite), and c defined below.

$$c \equiv \frac{\Sigma_s + \nu\Sigma_f}{\Sigma_t} \tag{1}$$

For these benchmarks, while the ratio of c is varied, Σ_t is always kept at unity. Along with other approximations, which vary from one benchmark to another, the mono-energetic approximation is the first step toward making these transport problems tractable. To get to the one group form, we assume neutrons scatter elastically from nuclei with infinite mass and thus do not lose energy. After integrating out energy we obtain the one group version of the transport equation [6]:

$$[\Omega \cdot \nabla + \Sigma(r, E_0)]\, \phi(r, \Omega) = \int_{4\pi} d\Omega' \Sigma_s(r, \Omega' \cdot \Omega, E_0)\phi(r, \Omega') + \frac{1}{4\pi}\nu(E_0)\Sigma_f(r, E_0) \int_{4\pi} d\Omega' \phi(r, \Omega') + Q(r, \Omega) \tag{2}$$

where $(\Omega \cdot \nabla)\phi(r, \Omega)$ represents neutrons streaming out of the volume, $\Sigma(r, E_0)\phi(r, \Omega)$ represents neutrons lost to absorption, $\int_{4\pi} d\Omega' \Sigma_s(r, \Omega' \cdot \Omega, E_0)\phi(r, \Omega')$ represents neutrons scattering within the volume, the third term represents neutrons born from fission, and $Q(r, \Omega)$ represents the source. Equation (2) has five dimensions and thus is still difficult to solve mathematically. Further simplifications are necessary in order to be able to reach a solution analytically. A reduction to 1-D geometry, and making artificial cross-sections which only include elastic scatter, capture, and fission neutron physics are common assumptions made in the derivation of these simplified forms of the transport equation.

RESULTS AND ANALYSIS

Professor Ganapol provided the FORTRAN codes that were used to solve modified versions of the mono-energetic transport equation semi-analytically, for the different boundary conditions and values of c. The same problems were set up in MCNP6, and the data was compared using a python script. For ease of comparison, the numbering of the plots coincide with the numbering in Barry Ganapol's book.

Infinite Medium Benchmark 3.1

For Benchmark 3.1 the transport equation that is solved is for mono-energetic neutrons in a homogeneous infinite medium, scattering without energy loss. The problem is solved in MCNP6 using a F2 flux tally for a beam and isotropic source.

Figure 1 shows both the calculated and benchmark scalar flux (top) and the calculated scalar flux divided by the analytic solution (bottom) as a function of position in the slab for an isotropic source at the origin. The solutions, generated by a version of MCNP6 equivalent to MCNP6.1.1, are within statistics everywhere except near the source, where errors are shown to be of the order of <10%. After running all of the benchmark problems, this effect is found in most problems near sources, boundaries, and high flux gradients. The divergence of the MCNP6.1.1 solution can be explained by the method which the F2 flux tally is calculated:

$$\phi = \frac{1}{A * W} \sum_{i=1}^{N} \frac{wgt_i}{|\mu|_i}, \quad (3)$$

where A is the surface area, W is the total source weight, wgt

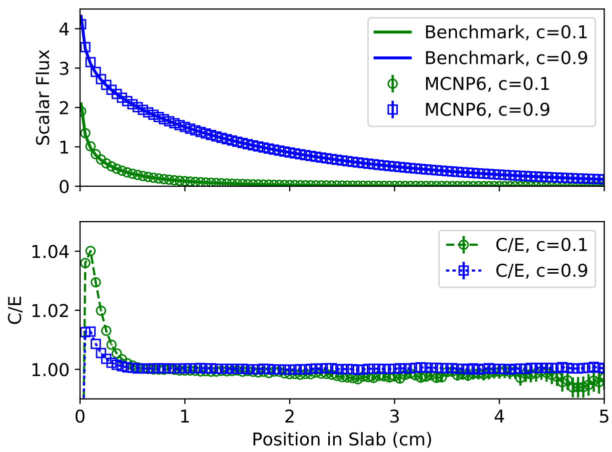

Fig. 1. Comparison of analytic results for Benchmark 3.1.2 with MCNP6 results for an isotropic source.

is the weight of the particle when crossing the surface, and $|\mu|$ is the absolute value of the cosine of the angle between the surface normal and the direction of the particle crossing the surface. As can be seen from Eq. 3 the F2 flux tally divides by the absolute value of the particle grazing angle with the surface. Below $|\mu| < .1$ MCNP6.1.1 makes a constant contribution to the F2 tally, in order to ensure that the variance of the flux is finite and to preserve good statistics. In the next release of the MCNP6 code, the grazing angle cutoff of $|\mu| < .1$ can be set with a user option or the new default grazing angle cutoff of $|\mu| < .001$ may be used. In Figure 2, the F2 flux tally divided by the semi-analytic solution is shown for both grazing angle cutoff parameters. Better agreement between the semi-analytic and MCNP solutions using the smaller grazing angle cutoff clearly shows the discrepancies are due to the assumptions made in the F2 flux tally at very small grazing angles.

Semi-Infinite Medium Benchmark 3.2 & 3.3

For Benchmark 3.2 and 3.3 the problem to be solved is mono-energetic neutron transport through a homogeneous material with vacuum boundary conditions either on one (half space 3.2) or both sides (finite slab 3.3) and an impinging beam on the left surface. The MCNP6 solutions for both of these benchmark suites are within statistics except near the source, which can be explained by the F2 tally contribution. Note that MCNP6 comparisons of the 3.2 benchmark problems have been discussed in Ref. 5.

Infinite Cylinder 3.4

Benchmark 3.4 deals with monoenergetic neutron transport in an isotropically scattering infinite cylinder with a vac-

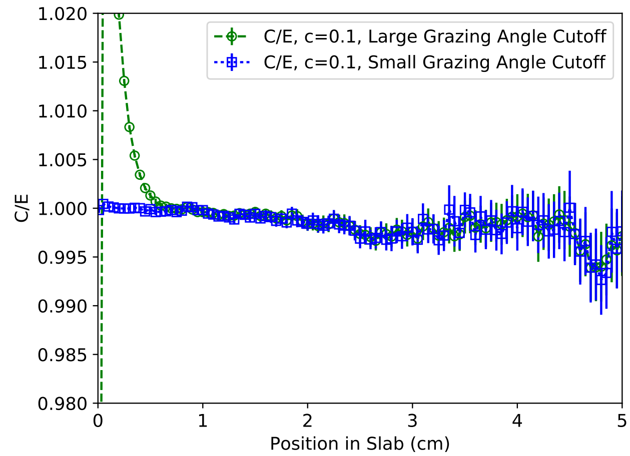

Fig. 2. Comparison of analytic results for Benchmark 3.1.2 with MCNP6 results for two grazing angle cutoffs.

uum boundary condition. As the neutrons enter the outside surface of the cylinder they initiate fission, which leads to the development of an internal flux profile. To compare MCNP6 results to the analytic "surrogate" flux (see Ref. 6 for details) solution a volume source must be used over the entire cylinder, with concentric infinite cylinders bounded by two reflecting surfaces. A flux F2 tally is then defined at each of the concentric cylinders to obtain the MCNP6 results. The flux shape for these problems is within statistics for most of the cylinder except near the edge, where there is a high flux gradient.

A variation on this benchmark included a criticality calculation of the infinite cylinder. By varying the value of c in Eq. 1, the critical radius of an infinite cylinder is calculated by Ganapol and compared to values reported in the literature [6, 7]. In the present work, using the c and critical radius values, the MCNP6 results for k_{eff} and the critical flux shape agree nicely with the benchmark results as can be seen by figure 3. Note that the results of surface flux tallies in the criticality calculations are not very sensitive to the grazing angle cutoff parameter compared with the other fixed-source results in the present work.

CONCLUSIONS

It is extremely important not only to properly set up the source, but to use the correct tallies as well, as can be seen from these cases. The approximations present in the F2 tally are the primary source of inaccurate results near the sources and boundaries where low grazing angles may be prevalent. To mitigate this discrepancy the smaller grazing angle cutoff can be used (available in the next version of MCNP6), or all of these problems could be reworked using a F4 volume flux tally with very narrow volume widths in order to compare to the point-wise semi-analytic solutions. It is evident that when the correct source definition and tallies are used, the MCNP6 results match the analytical solution within statistics.

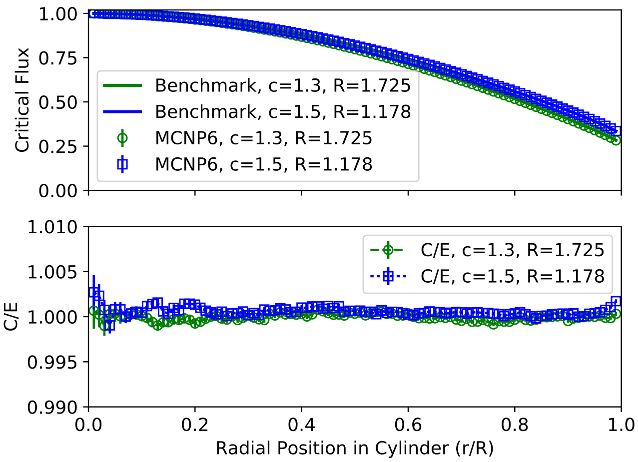

Fig. 3. MCNP6 values divided by the analytic solution for Benchmark 3.4.2 with a volume source for two values of c and radii.

ACKNOWLEDGMENTS

The authors would like to thank Professor Barry D. Ganapol for his gracious support in helping the authors learn and understand his benchmark textbook. This work was supported by the DOE Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.

REFERENCES

1. J. T. GOORLEY, M. JAMES, T. BOOTH, F. BROWN, J. BULL, J. COX, and J. DURKEE, "Initial MCNP6 Release Overview," *Nuclear Technology*, **180**, *3* (Jan 2012).
2. J. T. GOORLEY, "MCNP6.1.1-Beta Release Notes," *LA-UR-14-24680* (2014).
3. A. SOOD, D. K. PARSONS, and R. A. FORSTER, "Analytical Benchmark Test Set for Criticality Code Verification," *Prog. Nucl. Energy*, **42** (2003).
4. K. KOBAYASHI, N. SUGIMURA, and Y. NAGAYA, "3D radiation transport benchmark problems and results for simple geometries with void region," *Progress in Nuclear Energy*, **39**, *2* (2001).
5. B. GANAPOL and F. BROWN, "A Note on Boundary Conditions and Sources for Analytical Benchmarks," *proceeding of the 2015 ANS Winter Meeting*.
6. B. GANAPOL, *Analytical Benchmarks for Nuclear Engineering Applications - Case Studies in Neutron Transport Theory*, OECD Nuclear Energy Agency (2008).
7. C. E. SIEWERT, "The Critical Problem for an Infinite Cylinder," *Nuclear Science and Engineering*, **84**, *1* (Jun 1983).