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The MCNP6 Analytic Criticality Benchmark Suite

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INTRODUCTION

Analytical benchmarks provide an invaluable tool for verifying computer codes used to simulate neutron transport. Several collections of analytical benchmark problems [1-4] are used routinely in the verification of production Monte Carlo codes such as MCNP® [5,6].

Verification of a computer code is a necessary prerequisite to the more complex validation process. The verification process confirms that a code performs its intended functions correctly. The validation process involves determining the absolute accuracy of code results vs. nature. In typical validations, results are computed for a set of benchmark experiments using a particular methodology (code, cross-section data with uncertainties, and modeling) and compared to the measured results from the set of benchmark experiments. The validation process determines bias, bias uncertainty, and possibly additional margins. Verification is generally performed by the code developers, while validation is generally performed by code users for a particular application space.

The VERIFICATION_KEFF suite of criticality problems [1,2] was originally a set of 75 criticality problems found in the literature for which exact analytical solutions are available. Even though the spatial and energy detail is necessarily limited in analytical benchmarks, typically to a few regions or energy groups, the exact solutions obtained can be used to verify that the basic algorithms, mathematics, and methods used in complex production codes perform correctly. The present work has focused on revisiting this benchmark suite. A thorough review of the problems resulted in discarding some of them as not suitable for MCNP benchmarking. For the remaining problems, many of them were reformulated to permit execution in either multigroup mode or in the normal continuous-energy mode for MCNP. Execution of the benchmarks in continuous-energy mode provides a significant advance to MCNP verification methods.

REVISIONS TO THE VERIFICATION_KEFF SUITE

The VERIFICATION_KEFF verification suite has traditionally included 75 problems that were run as multigroup problems with MCNP. For the current work, the verification suite has been completely revised and reconfigured. New utility tools were developed to make it quick and easy to construct either multigroup ACE files or continuous-energy ACE files for use with the analytic test problems [7]. All of the problems were set up to use either multigroup or continuous-energy ACE files.

Review of Problem Suitability

A review of the 75 analytic problems was conducted, resulting in the following modifications to the suite:

- Problems 34, 37, 42, 43, and 71 included anisotropic P_1 scattering with $|\bar{\mu}| > 1/3$. This is nonphysical and yields a scattering PDF with negative values, which cannot be used in MCNP for random sampling of the cosine of the scattering angle. See [8] for details and discussion. Because of this, Problems 34, 37, 42, 43, and 71 were removed from the suite.
- Problems 33 and 35 involved anisotropic P_2 scattering, which is not currently handled by the scripts that construct the ACE files. For now, Problems 33 and 35 are not included in the suite. These problems may be included after enhancements to the data scripts.
- Problems 44 – 75 include group-to-group scattering. These problems are included in multigroup mode, but not for the continuous-energy mode for MCNP6.

The resulting set of 1-group or 1-speed problems 01-32, 36, 38-41 can be run as continuous-energy problems (e.g., “make ce01”) or as multigroup problems (e.g., “make mg01”).

Problems 44-70, 72-75 involve more than one group and can only be run in multigroup mode (e.g., “make mg72”).

On-the-fly ACE File Preparation

For multigroup problems, the *simple_ace_mg.pl* script [7] is used to construct the multigroup ACE file for each problem on-the-fly as needed. The multigroup ACE files are not stored permanently.

For continuous-energy problems, the *simple_ace.pl* script [7] is used to construct the continuous-energy ACE file for each problem on-the-fly as needed. The continuous-energy ACE files are not stored permanently.

The ACE file names for 1-speed or 1-group problems are listed in Table I, along with the parameters used as input to the *simple_ace.pl* and *simple_ace_mg.pl* scripts, and the Table number from [1] that was the original source for these parameters.

The ACE file names for multigroup problems are listed in Table II, along with the parameters used as input to the *simple_ace_mg.pl* script, and the Table number from [1] that was the original source for these parameters.

Benchmark Input Files

The input files for all of the problems were checked against [1,2], adding more significant digits when available. The names of the input files were changed, using for example "ce01" as the name of Problem 01 run in continuous-energy mode, and "mg01" as the name of Problem 01 in multigroup mode. XSn cards were used in each input file, so that an xsdir_mcnp6.1 file is not used.

The ACE files associated with each of the benchmark input files are listed in Table III.

The input files were modified so that each problem would run 100k neutrons/cycle, discarding 100 cycles, and running a total of 600 cycles, resulting in 50M active neutron histories for each problem.

The Makefile was modified to permit changing the KCODE card parameters on the make line, by specifying

NEUTRONS=n
DISCARD=n
CYCLES=n
KEFF=x

where n is an integer, and x is the value to use for the initial k_{eff} guess. The make target "more" was also added to permit continuation runs to reduce statistics.

The perl script to collect results, *get_results.pl*, was spruced-up to provide prettier output summaries.

Table I. Constants for 1-speed and 1-group Problems

ACE file	Nu	Fission	Capture	Scatter (P0)	Scatter (P1)	Total	Source [1]
99902.01c 99902.01m	3.24	0.081600	0.019584	0.225216	0	0.32640	Table 2
99902.02c 99902.02m	2.84	0.081600	0.019584	0.225216	0	0.32640	Table 2
99902.03c 99902.03m	0	0	0.032640	0.293760	0	0.32640	Table 2
99909.01c 99909.01m	2.70	0.065280	0.013056	0.248064	0	0.32640	Table 9
99909.02c 99909.02m	2.797101	0.065280	0.013056	0.248064	0	0.32640	Table 9
99909.03c 99909.03m	2.707308	0.065280	0.013056	0.248064	0	0.32640	Table 9
99909.04c 99909.04m	2.679198	0.065280	0.013056	0.248064	0	0.32640	Table 9
99909.05c 99909.05m	0	0	0.032640	0.293760	0	0.32640	Table 9
99913.01c 99913.01m	1.70	0.054628	0.027314	0.464338	0	0.54628	Table 13
99913.02c 99913.02m	0	0	0.054628	0.491652	0	0.54628	Table 13
99917.01c 99917.01m	2.50	0.06922744	0.01013756	0.328042	0	0.407407	Table 17
99917.02c 99917.02m	0	0	4.6512e-4	0.23209488	0	0.23256	Table 17
99917.03c 99917.03m	0	0	0	0.086368032	0	0.086368032	Table 17
99921.01c 99921.01m	2.50	0.266667	0	0.733333	0	1.0	Table 21
99921.02c 99921.02m	2.50	0.266667	0	0.733333	0.20	1.0	Table 21
99923.01c 99923.01m	2.70	0.065280	0.013056	0.248064	0.042432	0.32640	Table 23
99925.01c 99925.01m	1.808381	0.054628	0.027314	0.464338	0.056312624	0.54628	Table 25
99925.02c 99925.02m	1.841086	0.054628	0.027314	0.464338	0.112982569	0.54628	Table 25

Table II. Constants for Multigroup Problems

ACE file	Chi	Nu	Fission	Capture	Scatter (P0)	Scatter (P1)	Total	Source [1]
99927.01m	0.575 0.425	3.10 2.93	0.0936 0.08544	0.00480 0.0144	0.0792 0.0432 0.0 0.23616	0 0 0 0	0.2208 0.3360	Tables 27, 28
99930.01m	0.575 0.425	2.70 2.50	0.06192 0.06912	0.00384 0.01344	0.078240 0.0720 0.0 0.26304	0 0 0 0	0.2160 0.3456	Tables 30, 31
99933.01m	1.0 0.0	0.0 2.830023	0.0 0.060706	0.000217 0.003143	0.247516 0.020432 0.0 1.213127	0 0 0 0	0.268165 1.276976	Tables 33, 34
99936.01m	1.0 0.0	2.50 2.50	0.0010484 0.050632	0.0010046 0.025788	0.62568 0.029227 0.0 2.44383	0 0 0 0	0.65696 2.52025	Tables 36, 37
99940.01m	1.0 0.0	2.50 2.50	0.000836 0.029564	0.001104 0.024069	0.83892 0.04635 0.000767 2.9183	0 0 0 0	0.88721 2.9727	Tables 40, 41
99940.02m	1.0 0.0	2.50 2.50	0.001648 0.057296	0.001472 0.029244	0.83807 0.04536 0.00116 2.8751	0 0 0 0	0.88655 2.9628	Tables 40, 41
99940.03m	0 0	0 0	0 0	0.00074 0.018564	0.83975 0.04749 0.000336 2.9676	0 0 0 0	0.88798 2.9865	Tables 40, 41
99943.01m	1.0 0.0	1.004 2.50	0.61475 0.045704	0.0019662 0.023496	0.0 0.0342008 0.0 2.06880	0 0 0 0	0.650917 2.13800	Tables 43, 44
99943.02m	0 0	0 0	0 0	8.480293e-6 0.00016	0.1096742149 0.001000595707 0.0 0.36339	0 0 0 0	0.1106832906 0.36355	Tables 43, 44
99943.03m	0 0	0 0	0 0	4.97229e-4 0.0188	1.226381244 0.1046395340 0.0 4.35470	0 0 0 0	1.331518007 4.37350	Tables 43, 44
99946.01m	1.0 0.0	2.50 2.50	0.002817 0.097	0.0087078 0.02518	0.31980 0.0045552 0.0 0.42410	0 0 0 0	0.33588 0.54628	Tables 46, 47
99949.01m	1.0 0.0	2.50 2.50	0.0010484 0.050632	0.0010046 0.025788	0.62568 0.029227 0.0 2.44383	0.27459 0.0075737 0.0 0.83318	0.65696 2.52025	Tables 49, 50
99953.01m	1.0 0.0	2.50 2.50	0.0028172 0.097	0.0087078 0.02518	0.31980 0.004555 0.0 0.42410	0.06694 -0.0003972 0.0 0.05439	.33588 0.54628	Tables 53, 54
99956.01m	0.96 0.04 0.0	3.00 2.50 2.00	0.006 0.060 0.90	0.006 0.040 0.20	0.024 0.171 0.033 0.0 0.60 0.275 0.0 0.0 2.0	0 0 0 0 0 0 0 0 0	0.240 0.975 3.10	Tables 56,57,58
99959.01m	0.48 0.02 0.0 0.0 0.02 0.48	3.0 2.50 2.0 2.0 2.50 3.0	0.006 0.060 0.90 0.90 0.060 0.006	0.006 0.040 0.20 0.20 0.040 0.006	0.024 0.171 0.033 0.0 0.0 0.0 0.0 0.60 0.275 0.0 0.0 0.0 0.0 0.0 2.0 0.0 0.0 0.0 0.0 0.0 0.0 2.0 0.0 0.0 0.0 0.0 0.0 0.275 0.60 0.0 0.0 0.0 0.0 0.033 0.171 0.024	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0.240 0.975 3.10 3.10 0.975 0.240	Tables 59 - 64

RESULTS

Table V provides a comparison of MCNP6.2-pre results with the exact analytic results for the 1-speed ("ce") and 1-group ("mg") problems in the **VERIFICATION_KEFF** suite. For this comparison, the pre-release development version of MCNP6.2 was used, running 50M active neutrons on each problem. The results are shown as (C/E-1), the fractional difference between computed and exact results, in units of pcm (1 pcm = 0.00001), showing that MCNP6 is accurate to within 3±3 pcm.

Table VI provides a comparison of MCNP6.2-pre results with the exact analytic results for the multigroup problems in the **VERIFICATION_KEFF** suite. Problems 44-70,72, and 73 are 2-group problems; problem74 is a 3-group problem; and problem 75 is a 6-group problem.

SUMMARY

The changes noted above were made to the MCNP6 Git repository and will be included with the upcoming MCNP6.2 release.

It should be noted that previous usage of the **VERIFICATION_KEFF** suite made use of different coding in MCNP6, the multigroup coding, that is never used in realistic nuclear criticality safety calculations. With the above modifications to the suite, the problems can now exercise the continuous-energy coding portions of MCNP6, the same coding that is used in realistic nuclear criticality safety calculations. (Of course, the continuous-energy physics in this suite is limited to 1-speed problems with elastic scattering, but at least the overall flow of the calculation stays involves the standard continuous-energy portions of MCNP6.)

Table III. ACE Files for 1-speed & 1-group Problems

mg01:	99902.01m		
ce01:	99902.01c		
mg02:	99902.01m		
ce02:	99902.01c		
mg03:	99902.01m	99902.03m	
ce03:	99902.01c	99902.03c	
mg04:	99902.01m	99902.03m	
ce04:	99902.01c	99902.03c	
mg05:	99902.02m		
ce05:	99902.02c		
mg06:	99902.02m		
ce06:	99902.02c		
mg07:	99902.02m		
ce07:	99902.02c		
mg08:	99902.02m		
ce08:	99902.02c		
mg09:	99902.02m	99902.03m	
ce09:	99902.02c	99902.03c	
mg10:	99902.02m	99902.03m	
ce10:	99902.02c	99902.03c	
mg11:	99909.01m		
ce11:	99909.01c		
mg12:	99909.01m		
ce12:	99909.01c		
mg13:	99909.01m		
ce13:	99909.01c		
mg14:	99909.01m		
ce14:	99909.01c		
mg15:	99909.02m		
ce15:	99909.02c		
mg16:	99909.02m	99909.05m	
ce16:	99909.02c	99909.05c	
mg17:	99909.03m		
ce17:	99909.03c		
mg18:	99909.03m	99909.05m	
ce18:	99909.03c	99909.05c	
mg19:	99909.04m		
ce19:	99909.04c		
mg20:	99909.04m	99909.05m	
ce20:	99909.04c	99909.05c	
mg21:	99913.01m		
ce21:	99913.01c		
mg22:	99913.01m		
ce22:	99913.01c		
mg23:	99913.01m		
ce23:	99913.01c		
mg24:	99913.01m		
ce24:	99913.01c		
mg25:	99913.01m	99913.02m	
ce25:	99913.01c	99913.02c	
mg26:	99913.01m	99913.02m	
ce26:	99913.01c	99913.02c	
mg27:	99913.01m	99913.02m	
ce27:	99913.01c	99913.02c	
mg28:	99913.01m	99913.02m	
ce28:	99913.01c	99913.02c	
mg29:	99917.01m		
ce29:	99917.01c		
mg30:	99917.01m	99917.02m	99917.03m
ce30:	99917.01c	99917.02c	99917.03c
mg31:	99921.01m		
ce31:	99921.01c		
mg32:	99921.02m		
ce32:	99921.02c		
ce36:	99923.01c		
mg36:	99923.01m		
ce38:	99925.01c		
mg38:	99925.01m		
ce39:	99925.01c		
mg39:	99925.01m		
ce40:	99925.02c		
mg40:	99925.02m		
ce41:	99925.02c		
mg41:	99925.02m		

Table IV. ACE Files for Multigroup Problems

mg44:	99927.01m	
mg45:	99927.01m	
mg46:	99927.01m	
mg47:	99930.01m	
mg48:	99930.01m	
mg49:	99930.01m	
mg50:	99933.01m	
mg51:	99933.01m	
mg52:	99933.01m	
mg53:	99936.01m	
mg54:	99936.01m	
mg55:	99936.01m	
mg56:	99940.01m	
mg57:	99940.02m	
mg58:	99940.01m	99940.03m
mg59:	99940.01m	99940.03m
mg60:	99940.01m	99940.03m
mg61:	99940.02m	99940.03m
mg62:	99943.01m	
mg63:	99943.01m	99943.02m
mg64:	99943.01m	99943.02m
mg65:	99943.01m	99943.03m
mg66:	99943.01m	99943.03m
mg67:	99946.01m	
mg68:	99946.01m	
mg69:	99946.01m	
mg70:	99949.01m	
mg72:	99953.01m	
mg73:	99953.01m	
mg74:	99956.01m	
mg75:	99959.01m	

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REFERENCES

1. A. Sood, R.A. Forster, D.K. Parsons, "Analytic Benchmark Test Set for Criticality Code Verification," *Prog. Nucl. Energy*, **42**, 55-106 (2003).

2. A. Sood, R.A. Forster, D.K. Parsons, "Analytic Benchmark Test Set for Criticality Code Verification", LA-13511 and LA-UR-01-3082 (2001).

3. K. Kobayashi, N. Sugimura, Y. Nagaya, “3-D Radiation Transport Benchmark Problems and Results for Simple Geometries with Void Regions”, OECD/NEA (2000).

4. B.D. Ganapol, “Analytical Benchmarks for Nuclear Engineering Applications – Case Studies in Neutron Transport Theory”, OECD Nuclear Energy Agency, NEA No. 6292 (2008).

5. J.T. Goorley, et al., "Initial MCNP6 Release Overview," *Nuclear Technology*, **180**, 298 (2012).

6. J.T. Goorley, "MCNP6.1.1-Beta Release Notes," LA-UR-14-24680 (2014).

7. F.B. Brown, “New Tools to Prepare ACE Cross-section Files for MCNP Analytic Test Problems”, LA-UR-16-xxxxx (2016).

8. F.B. Brown & N. Barnett, “One-group MCNP5 Criticality Calculations with Anisotropic Scattering”, *Trans. ANS* **98**, Anaheim CA, June 2008, LA-UR-08-0567 (2008).

Table V. MCNP6 Results vs. Exact Results for Analytic Criticality Problems, 1-speed & 1-group Problems

Case	Name	Analytic keff	MCNP_Multigroup C/E-1	std		MCNP Continuous Energy C/E-1	std	
01	PUa-1-0-IN	2.61290	-0 pcm	0		-0 pcm	0	
02	PUa-1-0-SL	1.00000	0	5		6	5	
03	PUa-H2O(1)-1-0-SL	1.00000	8	5	*	1	5	
04	PUa-H2O(0.5)-1-0-SL	1.00000	2	5		3	5	
05	PUb-1-0-IN	2.29032	-0	0		-0	0	
06	PUb-1-0-SL	1.00000	4	4		0	4	
07	PUb-1-0-CY	1.00000	-4	4	*	3	4	
08	PUb-1-0-SP	1.00000	6	4	*	6	4	*
09	PUb-H2O(1)-1-0-CY	1.00000	-3	4		5	4	
10	PUb-H2O(10)-1-0-CY	1.00000	5	4		5	5	
11	Ua-1-0-IN	2.25000	0	0		0	0	
12	Ua-1-0-SL	1.00000	6	4	*	-3	4	
13	Ua-1-0-CY	1.00000	4	4		3	4	
14	Ua-1-0-SP	1.00000	1	4		-5	4	*
15	Ub-1-0-IN	2.33092	0	0		0	0	
16	Ub-H2O(1)-1-0-SP	1.00000	-2	4		-1	4	
17	Uc-1-0-IN	2.25608	0	0		0	0	
18	Uc-H2O(2)-1-0-SP	1.00000	-1	4		0	4	
19	Ud-1-0-IN	2.23267	-0	0		-0	0	
20	Ud-H2O(3)-1-0-SP	1.00000	4	4		7	4	*
21	UD2O-1-0-IN	1.13333	-0	0		-0	0	
22	UD2O-1-0-SL	1.00000	3	2		0	2	
23	UD2O-1-0-CY	1.00000	-1	2		-5	2	**
24	UD2O-1-0-SP	1.00000	1	3		-4	2	**
25	UD2O-H2O(1)-1-0-SL	1.00000	2	2		-2	2	*
26	UD2O-H2O(10)-1-0-SL	1.00000	-5	2	**	1	2	
27	UD2O-H2O(1)-1-0-CY	1.00000	4	2	*	-1	2	
28	UD2O-H2O(10)-1-0-CY	1.00000	0	2		3	2	
29	Ue-1-0-IN	2.18067	0	0		0	0	
30	Ue-Fe-Na-1-0-SL	1.00000	-1	5		7	4	*
31	PU-1-1-IN	2.50000	0	0		0	0	
32	PUa-1-1-SL	1.00000	8	5	*	7	5	*
36	Ua-1-1-CY	1.00000	2	4		-3	4	
38	UD2Oa-1-1-IN	1.20559	0	0		0	0	
39	UD2Oa-1-1-SP	1.00000	-2	3		2	3	
40	UD2Ob-1-1-IN	1.22739	-0	0		-0	0	
41	UD2Ob-1-1-SP	1.00000	8	3	**	6	3	*
		RMS Differences	3 pcm ± 3 pcm			3 pcm ± 3 pcm		

Table VI. MCNP6 Results vs. Exact for Multigroup Analytic Criticality Problems

Case	Name	Analytic keff	MCNP_Multigroup C/E-1	std	
44	PU-2-0-IN	2.68377	-1 pcm	0	***
45	PU-2-0-SL	1.00000	2	5	
46	PU-2-0-SP	1.00000	-1	4	
47	U-2-0-IN	2.21635	-0	0	
48	U-2-0-SL	1.00000	1	4	
49	U-2-0-SP	1.00000	-6	4	*
50	UAL-2-0-IN	2.66244	0	1	
51	UAL-2-0-SL	1.00000	20	8	**
52	UAL-2-0-SP	1.00000	14	9	*
53	URRa-2-0-IN	1.63145	0	1	
54	URRa-2-0-SL	1.00000	-3	5	
55	URRa-2-0-SP	1.00000	-4	6	
56	URRb-2-0-IN	1.36582	-0	0	
57	URRc-2-0-IN	1.63338	0	1	
58	URRb-H2Oa(1)-2-0-SL	1.00000	-7	4	
59	URRb-H2Oa(5)-2-0-SL	1.00000	-1	4	
60	URRb-H2Oa(IN)-2-0-SL	1.00000	-4	4	*
61	URRc-H2Oa(IN)-2-0-SL	1.00000	-4	5	
62	URRd-2-0-IN	1.03497	1	1	
63	URRd-H2Ob(1)-2-0-ISLC	1.00000	-4	2	**
64	URRd-H2Ob(10)-2-0-ISLC	1.00000	1	2	
65	URRd-H2Oc(1)-2-0-ISLC	1.00000	0	2	
66	URRd-H2Oc(10)-2-0-ISLC	1.00000	3	2	
67	UD2O-2-0-IN	1.00020	-1	4	
68	UD2O-2-0-SL	1.00000	-10	4	**
69	UD2O-2-0-SP	1.00000	-11	4	**
70	URRa-2-1-IN	1.63145	0	1	
72	UD2O-2-1-IN	1.00020	0	4	
73	UD2O-2-1-SL	1.00000	-7	4	*
74	URR-3-0-IN	1.60000	0	0	
75	URR-6-0-IN	1.60000	0		