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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.

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 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.

RESULTS

Table 1 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 2 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.)

ACKNOWLEDGMENTS

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

Case	Name	Analytic keff	MCNP_Multigroup C/E-1	MCNP_Multigroup std		MCNP Continuous Energy C/E-1	MCNP Continuous Energy 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 2. MCNP6 Results vs. Exact for Multigroup Analytic Criticality Problems

Case	Name	Analytic keff	MCNP_Multigroup C/E-1	MCNP_Multigroup 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		