LA-UR- 99-2566

Approved for public release; distribution is unlimited.

Title: VERIFICATION OF MCNP AND DANT/SYS WITH THE ANALYTIC BENCHMARK TEST SET

Author(s): D. K. Parsons
Avneet Sood
R. A. Forster
R. C. Little

Submitted to: Sixth International Conference on Nuclear Criticality Safety, September 20-24, 1999, Palais des Congres, Versailles, FRANCE

Los Alamos
NATIONAL LABORATORY

DISCLAIMER

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

VERIFICATION OF MCNP AND DANT/SYS WITH THE ANALYTIC BENCHMARK TEST SET

D. K. Parsons
Los Alamos National Laboratory
Group X-CI MS F663
Los Alamos, NM 87545
email: dkp@lanl.gov
fax: 505-665-5553
phone: 505-667-0504

Avneet Sood
North Carolina State University
Nuclear Engineering Department
Raleigh, NC 27695-7909

R. A. Forster
Los Alamos National Laboratory
Group X-CI MS F663 Los Alamos, NM 87545
email: raf@lanl.gov
fax: 505-665-5553
phone: 505-667-5777

R. C. Little
Los Alamos National Laboratory
Group X-CI MS F663
Los Alamos, NM 87545
email: rcl@lanl.gov
fax: 505-665-5553
phone: 505-665-3487

Introduction

The recently published analytic benchmark test set[1] has been used to verify the multigroup option of MCNP and also the deterministic DANT/sys series of codes for criticality calculations. All seventy-five problems of the test set give values for k_{eff} accurate to at least five significant digits. Flux ratios and flux shapes are also available for many of the problems. All seventy-five problems have been run by both the MCNP and DANT/sys codes and comparisons to k_{eff} and flux shapes have been made. Results from this verification exercise are given below.

High Precision Multigroup MCNP Calculations

Cross-section libraries for multigroup MCNP were generated with a locally developed utility program MAKEMG. Multigroup cross sections input by the user are converted into the appropriate MCNP library format. Anisotropic scattering is handled by an equally probable bin approach. Criticality calculations were typically carried out with 40,000 particles per cycle and 2,000 active cycles. The very large number of particles per cycle is necessary to suppress the known small negative bias in k_{eff} from the Monte Carlo power iteration method.[2] The large number of particle histories are also required to produce high-precision Monte Carlo confidence interval results.

High Precision DANT/sys Calculations

Deterministic codes like DANT/sys discretize both the spatial and angular variation of the flux in transport calculations. In order to analyze the high precision benchmarks, these discretization errors must be suppressed. Therefore a very large number of spatial mesh cells (1000's) and a very large number of angular ordinates (maximum allowed by the code) were used in the DANT/sys calculations. Furthermore, the most accurate types of quadrature (e.g., double P_n for slab geometry) and fix-ups for flux dip in curvilinear geometries[3] are also required for high precision. Fortunately, the benchmark problems are at most two-dimensional and deterministic calculations are very fast for one- and two-dimensions.

Code Issues Encountered During Verification

The representation of anisotropic scattering was found to be problematic. In four of the benchmark problems, the linearly anisotropic scattering is so forward peaked that the scattering cross section goes negative for back scattering. This negativity is caused by the truncation of the Legendre expansion of the scattering cross sections. For DANT/sys, any negative angular fluxes caused by the negative scattering are set to zero in a neutron conserving manner. In fact, such negative angular fluxes were seldom observed during verification. In MCNP, on the other hand, negative scattering cross sections are not allowed. For this test set, a KENO style and a maximum entropy approach were used[4] to change the scattering cross sections so as to be everywhere positive and yet still preserve the zeroth (Σ_s^{p0}) and the first ($\overline{\mu}$) moments of the scattering expansion. Only the shape and consequently, the higher moments, of the scattering cross section with respect to angle, were changed.

Some of the analytic results found during the literature search required a creative usage of MCNP and DANT/sys. Using an extended definition of $c = \frac{\upsilon\Sigma_f + \Sigma_s}{\Sigma_t}$, these particular analytic benchmarks give k_{eff} results for multiple values of $\overline{\mu}$. Since no information is given about the relative magnitudes of $\upsilon\Sigma_f$ and Σ_s, and since both MCNP and DANT/sys require some amount of $\upsilon\Sigma_f$ for a criticality calculation, it would appear that "anisotropic fission" would be required. However, for the case of only 1 group, appropriate cross-section modifications were derived and "anisotropic fission" was exactly modelled in both MCNP and DANT/sys.

Summary of Results

Apart from one of the anisotropic scattering cases mentioned above, all of the DANT/sys results matched the analytic results to a relative error of 0.001 to 0.00001. The worst results came from the 1D cyclindrical calculations because quadrature sets beyond S16 are not readily available. When the 1D cylindrical problems were transformed into 2D r-z geometry, where higher order Tchebychev-Legendre quadrature sets are available, then all of the DANT/sys results had relative k_{eff} errors less than 0.0001. The DANT results are given in Table I.

TABLE I:

Problem #	Problem ID	k_{eff}	True $_{keff}$
1	PUa-1-0-IN	2.61290	2.612903
2	PUa-1-0-SL	0.99999	1.000000
3	PUa-H2O(1)-1-0-SL	0.99997	1.000000
4	PUa-H2O(0.5)-1-0-SL	0.99999	1.000000
5	PUb-1-0-IN	2.29032	2.290323
6	PUb-1-0-SL	0.99999	1.000000
7	PUb-1-0-CY	1.00112	1.000000
7a	PUb-1-0-CY	1.00081	1.000000
7b	PUb-1-0-CY	1.00000	1.000000
8	PUb-1-0-SP	1.00001	1.000000
8a	PUb-1-0-SP	1.00001	1.000000
9	PUb-H2O(1)-1-0-CY	1.00143	1.000000
9a	PUb-H2O(1)-1-0-CY	1.00108	1.000000
9b	PUb-H2O(1)-1-0-CY	1.00108	1.000000
10	PUb-H2O(10)-1-0-CY	1.00137	1.000000
10a	PUb-H2O(10)-1-0-CY	1.00103	1.000000
11	Ua-1-0-IN	2.25000	2.250000
12	Ua-1-0-SL	0.99999	1.000000
13	Ua-1-0-CY	1.00093	1.000000
13a	Ua-1-0-CY	1.00067	1.000000
14	Ua-1-0-SP	1.00001	1.000000
14a	Ua-1-0-SP	1.00001	1.000000
15	Ub-1-0-IN	2.33091	2.330917
16	Ub-H2O(1)-1-0-SP	1.00001	1.000000
17	Uc-1-0-IN	2.25609	2.256083
18	Uc-H2O(2)-1-0-SP	1.00001	1.000000
19	Ud-1-0-IN	2.23266	2.232667
20	Ud-H2O(3)-1-0-SP	1.00001	1.000000
21	UD2O-1-0-IN	1.13333	1.133333
22	UD2O-1-0-SL	0.99999	1.000000
23	UD2O-1-0-CY	1.00001	1.000000
24	UD2O-1-0-SP	1.00000	1.000000
25	UD2O-H2O(1)-2-0-SL	0.99999	1.000000
26	UD2O-H2O(10)-2-0-SL	1.00000	1.000000
27	UD2O-H2O(1)-2-0-CY	1.00002	1.000000

TABLE 1 (cont.)

28	UD2O-H2O(10)-2-0-CY	1.00003	1.000000
29	Ue-1-0-IN	2.18066	2.180667
30	Ue-Fe-Na-1-0-SL	1.00000	1.000000
31	PU-1-1-IN	2.50000	2.500000
32	PUa-1-1-SL	1.00002	1.000000
33	PUa-1-2-SL	0.99998	1.000000
34	PUb-1-1-SL	0.99999	1.000000
35	PUb-1-2-SL	1.00003	1.000000
36	Ua-1-1-CY	1.00093	1.000000
36a	Ua-1-1-CY	1.00000	1.000000
37	Ub-1-1-CY	1.00085	1.000000
37a	Ub-1-1-CY	1.00000	1.000000
38	UD2Oa-1-1-IN	1.20558	1.205587
39	UD2Oa-1-1-SP	1.00000	1.000000
40	UD2Ob-1-1-IN	1.22739	1.227391
41	UD2Ob-1-1-SP	1.00000	1.000000
42	UD2Oc-1-1-IN	1.13093	1.130933
43	UD2Oc-1-1-SP	0.99999	1.000000
44	PU-2-0-IN	2.68376	2.683767
45	PU-2-0-SL	1.00000	1.000000
46	PU-2-0-SP	1.00010	1.000000
47	U-2-0-IN	2.21634	2.216349
48	U-2-0-SL	1.00000	1.000000
49	U-2-0-SP	1.00008	1.000000
50	UAL-2-0-IN	2.66174	2.661745
51	UAL-2-0-SL	0.99987	1.000000
52	UAL-2-0-SP	0.99992	1.000000
53	URRa-2-0-IN	1.63145	1.631452
54	URRa-2-0-SL	1.00000	1.000000
55	URRa-2-0-SP	1.00001	1.000000
56	URRb-2-0-IN	1.36582	1.365821
57	URRc-2-0-IN	1.63337	1.633380
58	URRb-H2Oa(1)-2-0-SL	0.99999	1.000000
59	URRb-H2Oa(5)-2-0-SL	0.99999	1.000000
60	URRb-H2Oa(IN)-2-0-SL	0.99999	1.000000
61	URRc-H2Oa(IN)-2-0-SL	0.99996	1.000000
62	URRd-2-0-IN	1.03497	1.034970
63	URRd-H2Ob(1)-2-0-ISLC	0.99997	1.000000
64	URRd-H2Ob(20)-2-0-ISL	0.99999	1.000000
65	URRd-H2Oc(1)-2-0-ISLC	0.99999	1.000000
66	URRd-H2Oc(10)-2-0-ISL	1.00000	1.000000
67	UD2O-2-0-IN	1.00019	1.000196
68	UD2O-2-0-SL	0.99997	1.000000
69	UD2O-2-0-SP	0.99997	1.000000

TABLE I (cont.)

70	URRa-2-1-IN	1.63145	1.631452
71	URRa-2-1-SL	0.99967	1.000000
72	UD2O-2-1-IN	1.00019	1.000196
73	UD2O-2-1-SL	1.00000	1.000000
74	URR-3-0-IN	1.60000	1.600000
75	URR-6-0-IN	1.60000	1.600000

MCNP k_{eff} results were converged to a standard deviation no larger than 0.0001. The k_{eff} confidence intervals had the expected coverage rates for the seventy-one problems without negative scattering. Forty-six problems had 68% one sigma confidence intervals that included the precise k_{eff} result. The 95% two sigma confidence intervals included the precise k_{eff} in sixty-eight problems. The largest number of standard deviations a mean k_{eff} was from the precise k_{eff} was 2.4 (98.5% confidence interval). The means were about equally distributed above and below the precise k_{eff} value. The results are given below in Table II.

TABLE II

Problem #	Problem ID	Combined k_{eff}	SD	# of SD	True k_{eff}
1	PUa-1-0-IN	2.61290	0.00000	0.000	2.612903
2	PUa-1-0-SL	1.00001	0.00008	0.125	1.000000
3	PUa-H2O(1)-1-0-SL	1.00000	0.00009	0.000	1.000000
4	PUa-H2O(0.5)-1-0-SL	1.00002	0.00009	0.222	1.000000
5	PUb-1-0-IN	2.29032	0.00000	0.000	2.290323
6	PUb-1-0-SL	1.00001	0.00007	0.143	1.000000
7	PUb-1-0-CY	1.00000	0.00007	0.000	1.000000
8	PUb-1-0-SP	1.00009	0.00007	1.286	1.000000
9	PUb-H2O(1)-1-0-CY	0.99999	0.00007	-0.143	1.000000
10	PUb-H2O(10)-1-0-CY	1.00009	0.00007	1.286	1.000000
11	Ua-1-0-IN	2.25000	0.00000	0.000	2.250000
12	Ua-1-0-SL	1.00010	0.00008	1.250	1.000000
13	Ua-1-0-CY	1.00010	0.00007	1.429	1.000000
14	Ua-1-0-SP	0.99994	0.00007	-0.857	1.000000
15	Ub-1-0-IN	2.33092	0.00000	0.000	2.330917
16	Ub-H2O(1)-1-0-SP	1.00003	0.00007	0.429	1.000000
17	Uc-1-0-IN	2.25613	0.00017	0.276	2.256083
18	Uc-H2O(2)-1-0-SP	1.00003	0.00008	0.375	1.000000
19	Ud-1-0-IN	2.23266	0.00000	0.000	2.232667
20	Ud-H2O(3)-1-0-SP	1.00010	0.00008	1.250	1.000000
21	UD2O-1-0-IN	1.13333	0.00000	0.000	1.133333
22	UD2O-1-0-SL	1.00006	0.00004	1.500	1.000000
23	UD2O-1-0-CY	0.99997	0.00005	-0.600	1.000000
24	UD2O-1-0-SP	1.00012	0.00005	2.400	1.000000
25	UD2O-H2O(1)-2-0-SL	1.00006	0.00005	1.200	1.000000
26	UD2O-H2O(10)-2-0-SL	0.99998	0.00004	-0.500	1.000000
27	UD2O-H2O(1)-2-0-CY	1.00006	0.00004	1.500	1.000000

Problem #	Problem ID	Combined k_{eff}	SD	# of SD	True k_{eff}
28	UD2O-H2O(10)-2-0-CY	0.99997	0.00004	-0.750	1.000000

TABLE II (cont.)

Problem #	Problem ID	Combined k_{eff}	SD	# of SD	True k_{eff}
29	Ue-1-0-IN	2.18067	0.00000	0.000	2.180667
30	Ue-Fe-Na-1-0-SL	0.99997	0.00008	-0.375	1.000000
31	PU-1-1-IN	2.50000	0.00000	0.000	2.500000
32	PUa-1-1-SL	0.99987	0.00008	-1.625	1.000000
33	PUa-1-2-SL	0.99990	0.00008	-1.250	1.000000
34	PUb-1-1-SL	1.00255	0.00008	31.875	1.000000
35	PUb-1-2-SL	1.00009	0.00008	1.125	1.000000
36	Ua-1-1-CY	0.99985	0.00007	-2.143	1.000000
37	Ub-1-1-CY	1.06170	0.00007	881.429	1.000000
38	UD2Oa-1-1-IN	1.20559	0.00000	0.000	1.205587
39	UD2Oa-1-1-SP	1.00009	0.00005	1.800	1.000000
40	UD2Ob-1-1-IN	1.22739	0.00000	0.000	1.227391
41	UD2Ob-1-1-SP	1.00005	0.00005	1.000	1.000000
42	UD2Oc-1-1-IN	1.13093	0.00000	0.000	1.130933
43	UD2Oc-1-1-SP	0.99681	0.00005	-63.800	1.000000
44	PU-2-0-IN	2.68377	0.00002	0.150	2.683767
45	PU-2-0-SL	0.99995	0.00008	-0.625	1.000000
46	PU-2-0-SP	0.99997	0.00007	-0.429	1.000000
47	U-2-0-IN	2.21632	0.00002	-1.450	2.216349
48	U-2-0-SL	1.00001	0.00008	0.125	1.000000
49	U-2-0-SP	0.99990	0.00007	-1.429	1.000000
50	UAL-2-0-IN	2.66172	0.00020	-0.125	2.661745
51	UAL-2-0-SL	1.00002	0.00018	0.111	1.000000
52	UAL-2-0-SP	0.99991	0.00019	-0.474	1.000000
53	URRa-2-0-IN	1.63141	0.00006	-0.700	1.631452
54	URRa-2-0-SL	1.00013	0.00010	1.300	1.000000
55	URRa-2-0-SP	1.00018	0.00010	1.800	1.000000
56	URRb-2-0-IN	1.36583	0.00001	0.900	1.365821
57	URRc-2-0-IN	1.63353	0.00010	1.500	1.633380
58	URRb-H2Oa(1)-2-0-SL	0.99995	0.00007	-0.714	1.000000
59	URRb-H2Oa(5)-2-0-SL	1.00011	0.00007	1.571	1.000000
60	URRb-H2Oa(IN)-2-0-SL	1.00002	0.00007	0.286	1.000000
61	URRc-H2Oa(IN)-2-0-SL	0.99995	0.00009	-0.556	1.000000
62	URRd-2-0-IN	1.03497	0.00001	0.000	1.034970
63	URRd-H2Ob(1)-2-0-ISLC	0.99997	0.00004	-0.750	1.000000
64	URRd-H2Ob(20)-2-0-ISL	0.99999	0.00004	-0.250	1.000000
65	URRd-H2Oc(1)-2-0-ISLC	0.99998	0.00004	-0.500	1.000000
66	URRd-H2Oc(10)-2-0-ISL	1.00005	0.00003	1.667	1.000000
67	UD2O-2-0-IN	1.00018	0.00007	-0.229	1.000196
68	UD2O-2-0-SL	1.00005	0.00007	0.714	1.000000
69	UD2O-2-0-SP	1.00015	0.00007	2.143	1.000000
70	URRa-2-1-IN	1.63147	0.00001	1.800	1.631452

TABLE II (cont.)

Problem #	Problem ID	Combined k_{eff}	SD	# of SD	True k_{eff}
71	URRa-2-1-SL	1.00229	0.00009	25.444	1.000000
72	UD2O-2-1-IN	1.00017	0.00007	-0.371	1.000196
73	UD2O-2-1-SL	1.00011	0.00007	1.571	1.000000
74	URR-3-0-IN	1.59997	0.00006	-0.500	1.600000
75	URR-6-0-IN	1.60000	0.00001	0.000	1.600000

The two group plutonium cross sections were modified to incorporate different values of the alpha eigenvalue; specifically, -0.1, 0., 0.1, and 0.2 generations/shake. MCNP ran these problems in a fixed source mode with time-dependent tallies. The asymptotic decay or growth rates match the alpha values to 0.01 generations/shake, which is within statistics of the calculation.

Comparisons with the high precision scalar flux results were also made. The DANT/sys flux results agree with the high precision values, but the McNP flux results showed some errors. This was determined to be a result of the empirical adjustments made to the F2 surface tallies for grazing angle crossings.

Conclusions

The verification activities on both DANT and MCNP were useful and provide confirmation that both codes are solving the k_{eff} eigenvalue problem correctly for multigroup cross sections.

References

1. A. Sood, R. A. Forster, and D. K. Parsons, "Analytical Benchmark Test Set for criticality Code Verification," LA–13511, Los Alamos National Laboratory, (1999).

2. E. M. Gelbard and R. Prael,, "Computations of Standard Deviations in Eigenvalue Calculations," Progress in Nuclear Energy, **24**, p. 237, (1990).

3. J. E. Morel and G. R. Montry, "Analysis and Elimination of the Discrete-Ordinates Flux Dip," Transport Theory and Statistical Physics, Vol. 13, No. 5, pp. 615-633, (1984).

4. D. K. Parsons, A Sood, R. A. Forster, and R. C. Little, "An Analuytic Benchmark Test Set for Criticality Code Verification and Its Application to MCNP and DANT/SYS," accepted for publication at the International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis, Madrid, Spain, (1999).