New Version of the MCNP Analytic Criticality Benchmark Suite

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Abstract

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Analytical benchmarks provide an invaluable tool for verifying computer codes used to simulate neutron transport. Several collections of analytical benchmark problems are used routinely in the verification of production Monte Carlo codes such as MCNP.

The VERIFICATION_KEFF suite of criticality problems was originally a set of 75 criticality problems found in the literature for which exact analytical solutions are available. 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 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.

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Outline

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Analytic Benchmarks

Verification & Validation

- **From ANSI/ANS-8.24-2007, Validation of Neutron Transport Methods for Nuclear Criticality Safety Calculations:**
  - **Verification:** Confirm that the *computer code system* correctly performs numerical calculations.
  - **Validation:** Quantify the suitability of the a computer code system for use in nuclear criticality safety analyses (e.g., establish the *bias* and *bias uncertainty*)

- **Verification, by code developers:**
  - ➜ Compare code results with analytic benchmarks (exact)
  - Compare code results with other more accurate codes (none...)
  - Compare code results with other similar codes (MCNP, Keno, ...)

- **Validation, by code developers:**
  - Compare code to benchmark experiments, for broad range

- **Validation, by end-users:**
  - Compare code to benchmark experiments, for specific range, set of benchmarks neutronically similar to applications

Analytical Benchmarks

- **Analytical benchmarks are an invaluable tool for verifying computer codes used to simulate neutron transport.**
  - Several collections of analytical benchmark problems are used routinely in the verification of production Monte Carlo codes such as MCNP
  - The spatial and energy detail is necessarily limited, typically to a few regions or energies
  - However, the exact solutions obtained can be used to verify basic algorithms, mathematics, and methods used in complex production codes
  - Verification of a computer code is a necessary prerequisite to the more complex validation process
  - Validation involves comparing the entire methodology of a code, cross-section data (with uncertainties), and modeling to results from a set of benchmark experiments

MCNP Verification & Validation Suites for Criticality

Verification Suites

- REGRESSION
  - 161 code test problems
  - Run by developers for QA checking
- VERIFICATION_KEFF
  - 75 analytic benchmarks (0-D and 1-D)
  - Exact solutions for k_{eff}
  - Past – multigroup,
    New – continuous-energy
- VERIFICATION_GENTIME
  - 10 benchmarks (analytic or comparisons to Partisn) for reactor kinetics parameters
- KOBAYASHI
  - 6 void & duct streaming problems, with point detectors, exact solutions
- Ganapol Benchmarks [in progress]
  - Exact, semi-analytic benchmark problems
  - Fixed source, not criticality
- Gonzales Benchmark [in progress]
  - Exact analytic benchmark with elastic scatter, including free-gas scatter

Validation Suites

- VALIDATION_CRITICALITY
  - 31 ICSBEP Cases
  - Too small a suite for serious V&V
  - Today, used for
    - Code-to-code verification, with real problems & data
    - Compiler-to-compiler verification, with real problems & data
    - Timing tests for optimizing MCNP coding & threading
- VALIDATION_CRIT_EXPANDED
  - 119 ICSBEP Cases
  - Broad-range validation, for developers
- VALIDATION_CRIT_WHISPER
  - 1101 ICSBEP Cases
  - Used with Whisper methodology for serious validation
  - Will be expanded, as time permits

Revisions to the VERIFICATION_KEFF Benchmark Suite

Review of Problem Suitability (1)

- **VERIFICATION_KEFF Suite**
  - **Technical basis**
    - A. Sood, R.A. Forster, D.K. Parsons, "Analytic Benchmark Test Set for Criticality Code Verification", *Prog. Nucl. Energy*, 42, 55-106 (2003).
    - Compilation of 75 criticality problems from the literature with exact analytic solutions to the criticality form of transport equation
      - 30 problems - 1-group, isotropic scatter
      - 13 problems - 1-group, anisotropic scatter
      - 26 problems - 2-group, isotropic scatter
      - 4 problems - 2-group, anisotropic scatter
      - 1 problem - 3-group, isotropic scatter
      - 1 problem - 6-group, isotropic scatter
  - **Used in the verification of all versions of MCNP5 & MCNP6**
  - **All problems were run using multigroup ACE cross-section files prepared by mgxs code (obsolete, unsupported)**
  - **Note that multigroup cross-sections are never used in criticality-safety calculations with MCNP**

Review of Problem Suitability (2)

Multigroup scatter in MCNP is modeled with equiprobable histograms in μ in the lab system (or equivalently, in CM system with infinite mass)

- **For problems with P_1 scattering where $|\bar{\mu}| > 1/3$,**
  - Part of the scatter PDF represents negative probability
  - This is nonphysical & not modeled by MCNP (not clear how to model…)
  - **Five of the benchmark problems (34, 37, 42, 43, 71) had $|\bar{\mu}| > 1/3$, & were removed from the benchmark suite**
- **For problems with P_2 scattering**
  - The utilities that construct the ACE files currently do not handle P_2 scattering (no check for negative portions of PDFs)
  - **The benchmark problems with P_2 scatter (33, 45) were removed, but may be reinstated in the future**
- **For problems with more than 1 group & group-to-group scattering**
  - **Problems 44-74 are only used in multigroup mode**
  - **Continuous-energy versions require mods to ACE utility routine**

Review of Problem Suitability (3)

Summary of benchmark problem suitability:

- **These 5 problems were removed permanently (bad P_1)**
  - **34, 37, 42, 43, 71**
- **These 2 problems were removed temporarily (P_2)**
  - **33, 35**
- **These 37 problems can be used for either continuous-energy or multigroup benchmark calculations**
  - **01-32, 36, 38-41**
- **These 31 problems can be used only for multigroup benchmark calculations**
  - **44-70, 72-75**

On-the-fly ACE File Preparation

- **Two utility scripts were written in perl for constructing ACE files for analytic benchmark problems**
  - **simple_ace.pl**
    - For constructing continuous-energy ACE files
    - Capture, fission, & elastic scatter only (no inelastic, n-2n, n-γ, etc.)
    - Cross-sections specified at E-points, with linear interpolation
    - Can specify mass & temperature, optional Doppler of scatter xsec
  - **simple_ace_mg.pl**
    - For constructing multigroup ACE files
    - Can be 1-group or multigroup with group-to-group scatter
  - **These are portable to Mac, Linux, & Windows**
  - **Easy to use, with minimal input**
  - **See mcnp.lanl.gov**

    F.B. Brown, "New Tools to Prepare ACE Cross- section Files for MCNP Analytic Test Problems", LA-UR-16-24290 (2016)

- **The Makefile for running the suite was modified to use these utilities to construct ACE files on-the-fly for each benchmark**

Benchmark Input Files

- **All benchmark input files for MCNP were reviewed & checked against the reference**
  - **In many cases, more significant digits were added to the inputs**

- **Input file names were changed**
  - **For continuous-energy inputs: ce01, ce02, …**
  - **For multigroup inputs: mg01, mg02, ...**

- **Default KCODE cards for all problems, for 50 M active neutrons:**

  kcode 100000 1.0 100 600

  For work in this talk, used *continue* runs for 250 M active neutrons

- **Optionally, can override default KCODE parameters on Make command line:**

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

- **Utility script collects Keff results from each output file**

Results

MCNP6 Analytic Criticality Verification

How accurate is MCNP6 if cross-sections & dimensions are exact ?

VERIFICATION_KEFF

- **A. Sood, R.A. Forster, D.K. Parsons, "Analytic Benchmark Test Set for Criticality Code Verification", *Prog. Nucl. Energy*, 42, 55-106 (2003). Also, LA-UR-01-3082, from mcnp.lanl.gov**
- **37 problems run using multigroup & continuous-energy**
- **31 problems run using multigroup only**
- **250 M active neutrons for all problems**
- **First time ever that this suite has been run using the continuous-energy physics routines in MCNP (previously, multigroup only)**
- **Results match exact analytic solutions within 0.00003 +- 0.00003**

MCNP6 Criticality Results vs Exact Results – MG & CE

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	

1 pcm = 0.00001

MCNP6 Criticality Results vs Exact Results – MG Only

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	0	
	RMS Differences		3 pcm	±3 pcm	

2 groups: 44-70, 72, 73
3 groups: 74
6 groups: 75

1 pcm = 0.00001

Conclusions

- **Analytical benchmarks are an invaluable tool for code developers**
  - **Exact results to compare to**
  - **Can test many – but not all - code features**
    - Yes – geometry, elastic scatter, tallies, point detectors, k-eff iterations, ...
    - No – inelastic scattering, S(a,b), unresolved resonances, ...
  - **Need to extend some of the analytical benchmarks to include varying cross-sections (with energy)**

- **Results match exact values to 0.00003 ± 0.00003 (RMS)**

- **Significant technical advance:**
  - **Using same continuous-energy coding in MCNP that is used for realistic nuclear criticality safety calculations**
  - **Of course, the continuous-energy physics in this suite is limited to 1-speed problems with elastic scattering**
  - **But, the overall flow of the calculation uses the standard continuous-energy portions of MCNP6**

Questions ?

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