Verification of MCNP6.1, MCNP6.1.1, and MCNP6.2-pre for Criticality Safety Applications

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Abstract

Verification of MCNP6.1, MCNP6.1.1, and MCNP6.2-pre for Criticality Safety Applications

Forrest Brown, Michael Rising
Monte Carlo Methods, Codes, & Applications, LANL

Several suites of verification/validation benchmark problems were run in early 2016 to verify that MCNP6.1, MCNP6.1.1, and MCNP6.2-pre are performing correctly for nuclear criticality safety (NCS) applications. MCNP6.1 is the production version of MCNP released in 2013; MCNP6.1.1 is the update released in 2014; MCNP6.2-pre is the pre-release development version of MCNP6.2, which is targeted for release in the near future. All versions of MCNP6 include all of the standard features for NCS calculations that have been available for the past 15 years, along with new features for sensitivity- uncertainty based methods for NCS validation. Results from the benchmark suites were compared with results from previous verification testing

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Outline

US DOE-NNSA Nuclear Criticality Safety Program – What have we done for you lately ?

– MCNP6 Status

– Methodology & Background
  - Analytic Criticality Suites
  - Criticality Validation Suites
  - Fortran Compiler Issues

– Testing Results
  - VERIFICATION_KEFF Suite
  - VALIDATION_CRITICALITY Suite
  - VALIDATION_CRIT_EXPANDED Suite

– Summary & Conclusions

MCNP6 Status

MCNP6 Status (1)

- **MCNP releases by RSICC**

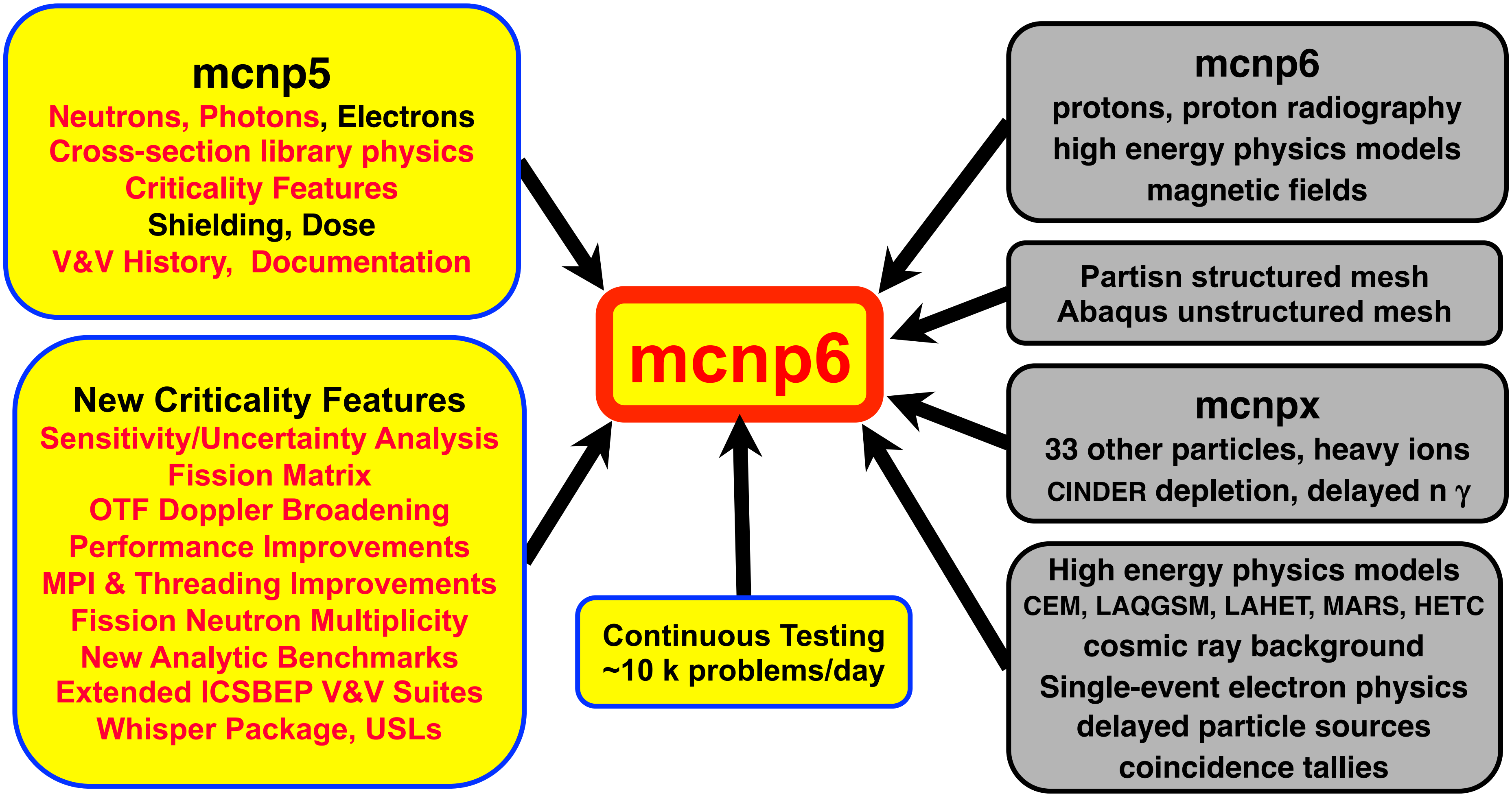
MCNP5	**– 2003-2013, R.I.P.**
MCNP6.1	**– 2013, production version**
MCNP6.1.1	**– 2014, same criticality, faster, beta features for DHS**
MCNP6.2	**– 2017, will include Whisper code & benchmarks**

Nuclear Data	**– ENDF/B-VII.1 data, updates, & older data**
Reference Collection	**– 700^{+} technical reports**
V&V Test Collection	**– 1500^{+} test problems**

12,000^{+}	**copies of MCNP5 distributed by RSICC**
8,000^{+}	**copies of MCNP6 distributed by RSICC**

- **MCNP6 usage on HPC systems at LANL**
  - **MCNP6 is used for about 1,000,000 hours / month.**
  - **Criticality safety accounts for 10-20% of usage.**

MCNP6 Status (2)



mcnp5 – 100 K lines of code
mcnp6 – 500 K lines of code

MCNP6 Status (3)

- MCNP6.2 new features
  - Longer input lines, up to 128 characters
  - Longer command-line, to support 256-character filenames
  - Bug fixes
    - Coincident surfaces for rotated universe/fill (25 year old bug)
    - Rare S(alpha,beta) sampling error (due to roundoff)
  - Features for criticality
    - Analytic criticality benchmarks now use continuous-energy physics
    - Warning message regarding bias if using < 10,000 neutrons/cycle
    - Same performance (speed) as MCNP6.1.1 (2x MCNP6.1)
    - **Whisper** coding, benchmarks, scripts, & documentation
  - Many other bug fixes & features, for non-criticality problems

- Release status
  - In final stages of code reviews, feature reviews, & clean up
  - Final documentation, release testing, & installers soon
  - Expected release to RSICC: late-2016 or early 2017

Methodology & Background

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

Verification & Validation

We do a lot of verification/validation work - all the time:

MCNP Verification-Validation, 100+ reports on MCNP Website

Verification of MCNP6.1, MCNP6.1.1, and MCNP6.2-pre for Criticality Safety Applications, LA-UR-16-24308 (2016)

The MCNP6 Analytic Criticality Benchmark Suite, LA-UR-16-24255 (2016)

New Version of the MCNP Analytic Criticality Benchmark Suite, LA-UR-16-24254 (2016)

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

MCNP6 Optimization & Testing for Criticality Safety Calculations, LA-UR-15-20422 (2015)

MCNP Verification & Validation, LA-UR-15-27015 (2015)

Validation of MCNP6.1 for Criticality Safety of Pu-Metal, -Solution, and -Oxide Systems, LA-UR-14-23352 (2014)

Verification of MCNP6.1 & MCNP6.1.1 for Criticality Safety Applications, LA-UR-14-22480 (2014)

Verification of MCNP5-1.60 and MCNP6.1 for Criticality Safety Applications, LA-UR-13-22196 (2013)

Verification of MCNP5-1.60 and MCNP6-Beta-2 for Criticality Safety Applications, LA-UR-12-210 (2012)

MCNP5-1.60 Release & Verification, LA-UR-11-00230 (2011)

ENDF/B-VII.1 Neutron Cross Section Data Testing with Critical Assembly Benchmarks & Reactor Experiments, Nuclear Data Sheets, Vol 112, No. 12, 2997-3036 [LA-UR-11-11271] (2011)

An Expanded Criticality Validation Suite for MCNP, ICNC-2011, LA-UR-11-04170 (2011)

Verification of MCNP5-1.60, LA-UR-10-05611 (2010).

MCNP Verification & Validation Suites for Criticality

See other paper at this meeting: Brown, New Version of the MCNP Analytic Criticality Benchmark Suite

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

Testing Methodology

- **Validation Suites**
  - **All calculations used ENDF/B-VII.1 cross-sections**
  - **Continuous S(alpha,beta) physics, not old discrete treatment**
    - **MCNP6.1 had a small, rare error in dealing with the continuous S(α,β) data:**
      - For some S(α,β) datasets at the very lowest energies (typically 10^{-5} – 10^{-4} eV), NJOY lumps together scattering probabilities smaller than 10^{-6}. MCNP6.1 did not handle that properly.
      - This problem was fixed in MCNP6.1.1 & MCNP6.2
      - **Insignificant impact on results, but should be some very minor differences for problems with thermal scattering between MCNP6.1 and later versions.**
- **Fortran Compilers**
  - **Intel-12 - MCNP6.1 & MCNP6.1.1, Intel-15,16,17 - MCNP6.2**
  - **Using different compilers always leads to minor differences due to roundoff**
  - **Roundoff differences due to the noncommutative and nonassociative nature of computer arithmetic, and the rearrangement of the order of operations by optimizing compilers.**
  - **Roundoff differences are <u>not</u> errors, but must be examined in detail**
- **Running strategy**
  - **All calculations performed with OpenMP threading, with 8-16 cpu-cores**
  - **Mac Pro, 12-core Xeon, 2 hyperthreads/core, OS X 10.9.5, 14 MCNP threads**
  - **Linux, 1 HPC node, 8 dual-core Xeons, Chaos linux, 16 MCNP threads**

Testing 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**

- **Compilation of 75 criticality problems from the literature with exact analytic solutions**

- **Complete overhaul in the past months**
  - Utilities to construct ACE files, multigroup & continuous-energy
  - Revised & checked xsecs & geometry (more digits in input, …..)

- **First time ever that this suite has been run using the continuous-energy physics routines in MCNP (previously, multigroup only)**

- **37 problems run using continuous-energy, 250 M neutrons each**
- **Results match exact analytic solutions within 0.00003 +- 0.00003**

MCNP6 Criticality Results vs Exact Results

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

Testing Results for VALIDATION_CRITICALITY Suite (1)

	610_Mac		611_Mac		620_Mac		610_Linux		611_Linux		620_Linux	
	keff	std	deltak	std	deltak	std	deltak	std	deltak	std	deltak	std
U233 Benchmarks												
JEZ233	1.0000	(5)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)
FLAT23	0.9974	(7)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)
UMF5C2	0.9960	(7)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)
FLSTF1	0.9845	(11)	0.0000	(15)	0.0000	(15)	0.0000	(15)	0.0000	(15)	0.0000	(15)
SB25	0.9997	(10)	0.0000	(14)	0.0000	(14)	0.0000	(14)	0.0000	(14)	0.0000	(14)
ORNL11	1.0018	(2)	0.0000	(4)	0.0000	(4)	0.0000	(4)	0.0000	(4)	0.0000	(4)
HEU Benchmarks												
GODIVA	0.9988	(5)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)
TT2C11	1.0009	(8)	0.0000	(11)	0.0000	(11)	0.0000	(11)	0.0000	(11)	0.0000	(11)
FLAT25	1.0034	(5)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)
GODIVR	0.9989	(7)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)
UH3C6	0.9957	(8)	0.0000	(11)	0.0000	(11)	0.0000	(11)	0.0000	(11)	0.0000	(11)
ZEUS2	0.9976	(7)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)
SB5RN3	0.9945	(13)	0.0000	(18)	0.0000	(18)	0.0000	(18)	0.0000	(18)	0.0000	(18)
ORNL10	1.0001	(4)	0.0000	(5)	0.0000	(5)	0.0000	(5)	0.0000	(5)	0.0000	(5)
IEU Benchmarks												
IMF03	1.0019	(5)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)
BIGTEN	0.9952	(5)	0.0000	(7)	0.0000	(7)	0.0000	(7)	0.0000	(7)	0.0000	(7)
IMF04	1.0082	(5)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)
ZEBR8H	1.0193	(5)	0.0000	(8)	-0.0011	(8)	-0.0011	(8)	-0.0011	(8)	-0.0011	(8)
ICT2C3	1.0023	(7)	0.0012	(9)	0.0012	(9)	0.0000	(9)	0.0012	(9)	0.0012	(9)
STACY36	0.9981	(5)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)
LEU Benchmarks												
BAWXI2	1.0025	(5)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)
LST2C2	0.9960	(5)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)
Pu Benchmarks												
JEZPU	0.9990	(5)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)
JEZ240	0.9999	(5)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)
PUBTNS	0.9980	(7)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)
FLATPU	1.0004	(7)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)
THOR	0.9976	(5)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)
PUSH2O	1.0013	(8)	0.0000	(11)	0.0000	(11)	0.0000	(11)	0.0000	(11)	0.0000	(11)
HISHPG	1.0121	(5)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)	0.0000	(8)
PNL2	1.0050	(10)	0.0000	(14)	0.0000	(14)	0.0000	(14)	0.0000	(14)	0.0000	(14)
PNL33	1.0068	(7)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)	0.0000	(9)

Testing Results for VALIDATION_CRITICALITY Suite (2)

- **Performance**

	610_Mac	611_Mac	620_Mac	610_Linux	611_Linux	620_Linux
Threads:	14	14	14	16	16	16
Wall-clock:	20.1 min	12.6 min	12.5 min	18.8 min	10.1 min	10.4 min
Rel. Speed:	1.00	1.59	1.60	0.94	1.73	1.69

- **Differences**
  - **29 out of 31 problems agreed with all versions & all systems**
  - **ICT2C3:**
    - MCNP6.1 and MCNP6.1.1: Difference $< 2\sigma$
    - MCNP6.1.1 and MCNP6.2-pre: Agree, for both Mac & Linux
    - Difference was almost certainly due to the **S(a,b) bug fix**, not roundoff
  - **ZEBR8H:**
    - Mac: 6.1 & 6.1.1 agreed, 6.2 difference $< 2\sigma$
    - Linux: 6.1 & 6.1.1 & 6.2 agreed, but differ from Mac
    - Difference was almost certainly due to **roundoff**

MCNP6 – Performance History

Run Times for VALIDATION_CRITICALITY Suite on Various Computers

Computer	CPU Speed (GHz)	Mem. Speed (GHz)	Processors, Cores	MCNP Threads used	MCNP Version	Total Time (minutes)
MacBook 2010	2.7	1.1	1 - i7, 2 x 2 HT	4	mcnp6.1.1	88
MacBook 2013	3.0	1.6	1 - i7, 2 x 2 HT	4	mcnp6.1	62
				4	mcnp6.1.1	42
Mac Pro 2010	3.0	0.67	2 - Xeon, 4	8	mcnp6.1	44
				8	mcnp6.1.1	28
Windows 2012	2.7	1.3	2 - Xeon, 6	10	mcnp6.1.1	19
Mac Pro 2012	2.4	1.07	2 - Xeon, 4 x 2 HT	16	mcnp6.1.1	22
Mac Pro 2014	2.7	1.6	1 - Xeon, 12 x 2 HT	12	mcnp5-1.60	14
				12	mcnp6.1.1	14
				14	mcnp6.1.1	12 ⇐
				14	mcnp6.2	12 ⇐
HP Linux 2016	3.1	2.4	2 - Xeon, 12 x 2 HT	24	mcnp6.2	8 ⇐

MCNP6.2 preserves all performance improvements from MCNP6.1.1, and is much faster than MCNP6.1 & slightly faster than MCNP5

Runtimes are wall-clock for the entire suite of 31 problems, including cross-section I/O & output

Testing Results for VALIDATION_CRIT_EXPANDED Suite

119 ICSBEP experiment benchmarks, ENDF/B-VII.1 nuclear data

- MCNP6.1, MCNP6.1.1, & MCNP6.2 results matched for all 119 ICSBEP problems on both Mac & Linux

- Comments

  - This is very nice, but fortuitous
  - With a bug fix & compiler roundoff differences, some diffs are expected
  - If problems were run for very many more histories, some diffs would eventually appear
  - This is true for any MC code & any set of problems, if different computers or compilers are used
  - Nevertheless, these results make validation easy – no diffs

Testing Summary

For testing on Mac & Linux, with OpenMP threading:

VERIFICATION_KEFF Suite – analytic problems with exact K_{eff} results

- **6.1, 6.1.1, 6.2: Results match exact within 3 pcm ± 3 pcm**

VALIDATION_CRITICALITY Suite – 31 ICSBEP, ENDF/B-VII.1

- **6.1, 6.1.1, 6.2: 29 results match, 1 bug fix diff, 1 roundoff diff**

VALIDATION_CRIT_EXPANDED Suite – 119 ICSBEP, ENDF/B-VII.1

- **6.1, 6.1.1, 6.2: All results match**

These tests are also run occasionally on Windows, with similar results.

Conclusions

- All current versions of MCNP6 – 6.1, 6.1.1, 6.2 – perform correctly for the 3 suites of analytic benchmarks & ICSBEP problems

- MCNP6 testing is performed very frequently for criticality problems during all MCNP code development
  - New features for non-criticality problems are disallowed if they affect criticality results
  - Because it only takes 12 minutes to run the VALIDATION_CRITICALITY suite using threading, it is run daily or weekly during development
  - MCNP6 performance is also monitored, with corrections or optimization if criticality performance changes

- There are no technical or correctness issues to delay switching to the latest version of MCNP6
  - MCNP5 is no longer supported
  - Newer versions – can use continuous S(a,b) data (MCNP5 cannot)
  - Newer versions – better performance & use of computer resources
  - Newer versions – bug fixes (few, since neutronics is mature)
  - Newer versions – better support from developers

Questions ?

Comments on Geometry & Performance

- **There was a paper presented at the ANS 2016 Summer meeting:**

  Zywiec & Heinrichs, "A Solid of Revolution Time Study using COG11.1 and MCNP6.1"

  In it, they discussed the run times for MCNP6 & COG for problems that involved contour geometry. That is, a series of points are specified & connected, and the curve is revolved around the main axis. They reported results for the pu-met-fast-001 benchmark, where the sphere was divided into segments and represented as (1) a solid of revolution (a special geometry that COG supports), and (2) using cones to represent each of the bounding segments (for both COG & MCNP6). They varied the number of segments from 10 to 990.

  – For the worst case, 990 segments, they reported these runtimes:

  22 minutes - COG, solid of revolution

  795 minutes - COG, conical segments

  201 minutes - MCNP6, conical segments

- **The exact same problem was set up & run at LANL with the standard RSICC released MCNP611. Runtime:**

  1 minute - MCNP6, conical segments, 1 cpu (2.7 GHz Xeon, 12-core)

- **In addition, the paper incorrectly stated that MCNP6 does not support a "solid of revolution". It does in fact support axisymmetric surfaces defined by points, & it is easy to set up the problem using them.**

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Approved for public release; distribution is unlimited.

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