LA-UR-23-30469

Approved for public release; distribution is unlimited.

Title:	MCNP6.2 and MCNP6.3 Performance Comparison
Author(s):	Bull, Jeffrey S.
Intended for:	2023 MCNP User Symposium, 2023-09-18/2023-09-21 (Los Alamos, New Mexico, United States)
Issued:	2023-09-26 (Rev.1) (Draft)

Los Alamos NATIONAL LABORATORY

MCNP6.2 and MCNP6.3 Performance Comparison

Jeffrey Bull
XCP-3, MCNP Development Team

2023 MCNP® User Symposium

September 20, 2023

LA-UR-23-30469

MCNP®
MONTE CARLO N-PARTICLE

Introduction

MCNP6.3 was finalized in March 2023. Since the release of MCNP6.2 in February 2018, a great number of changes have been made to the source code. Many of these changes were significant, others not so much. All the source code files were modified.

One of the goals of the MCNP Development Team is to at least maintain the performance of MCNP during the development process.

This work will compare the performance of MCNP6.3 with MCNP6.2

Performance Improvements in 6.3

From “MCNP® Code Version 6.3.0 Release Notes”, LA-UR-22-33103

- Unstructured Mesh Improvements
- Cross Section Cache Array Improvement
- Burn-up Memory Reduction
- ACT card DG = line option
- New HDF5/XDMF Meshtal Format
- Improvements for non-uniform memory access (NUMA)
- X11 plotter: background plot window drawing

ACT card DG = line option

- The algorithm for the delayed-gamma (DG) exact line treatment was rewritten by Greg Mckinney.

- Elapsed time to run the test serially
  - MCNP6.2 – 9 hours
  - MCNP6.3 – 11 minutes
  - Factor of 50 performance improvement
- Memory Footprint reduced by half

Test input file

```
Test new DG=line method on the ACT card
1 0 -1     imp:p=1
2 0  1     imp:p=0

1 so 100

mode #  p
c
c Source
sdef par=d1 erg=0
c  SI/SP cards for 1580 radioactive nuclides
si1 L  2006 2008 3008 3009 4007 4010 4012 …
sp1 1 1579r
c
act DG=line FISSION=p NONFISS=p
nps 1e5
c
e0 1e-3 999i 20
f1:p 1
```

Performance Test Suite

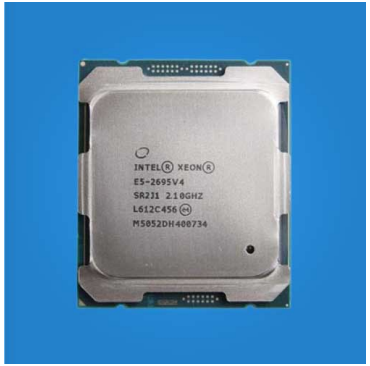
- 22 tests that cover various sections of the code
  - Kcode
    - Godiva
    - PWR initial core, 2D modle, 17 x 17 bundles, with and without 4096 x 4096 x 1 FMESH tally
  - Physics
    - Geometry: 25 concentric spheres out to16,265 m in air, with source points randomly distributed in a 900 m radius sphere
    - Modes: n, n p, n p e, p, p e
  - Tallies
    - F1, F2, F4, and F5, FMESH tallies: same geometry as the physics test, but in void instead of air
    - FIR, F8 (with and without variance reduction)
  - Other tests
    - Well log
    - Many surfaces: 1002 cells, 1001 surfaces
    - Lattice tracking: 1400 x 1400 x 51 lattice elements in void

Methodology

- CMake/CTest use to setup and run test suite
- Tested with the executables distributed by RSICC, except for Linux MCNP62 with MPI
- Parallel tests run with either all OpenMP threads or MPI processes
- Weak scaling
- Used number of histories per hour to compare performance
- Serial run times between 2 and 4 minutes

MCNP 6.2 and 6.3 Comparison: Linux -- Serial

- Linux RedHat 7.9
- Intel Xeon(R) CPU E5-2695 v4 @ 2.10GHz (Broadwell)
  - 2 CPUs
  - 18 cores/CPU
  - 36 threads
  - 2 NUMA nodes, one per CPU



Test Name	M histories per hour MCNP6.2	MCNP6.3	63 / 62 Ratio
boston_lattice	42.35	40.68	0.96
godiva	323.57	344.88	1.07
manysurfaces	33.33	41.38	1.24
mode_n_air	24.49	23.53	0.96
mode_np_air	13.24	13.64	1.03
mode_npe_air	1.15	1.10	0.96
mode_p_air	55.38	50.70	0.92
mode_pe_air	1.64	1.52	0.93
pwr2d_whole	18.31	17.86	0.98
tally_void_f1	266.67	264.71	0.99
tally_void_f2	262.77	257.14	0.98
tally_void_f4	255.32	246.58	0.97
tally_void_f5	340.16	324.81	0.95
tally_void_fmesh	268.66	258.99	0.96
tally_void_ref	425.20	421.88	0.99
tally_fir	0.0025	0.003	1.20
tally_kcode_fmesh	11.59	11.43	0.99
tally_pht	170.27	158.49	0.93
tally_phtvr	4.47	4.65	1.04
well_log	25.90	23.68	0.91
		Minimum	0.91
		Maximum	1.24
		Average	1

MCNP 6.2 and 6.3 Comparison – Linux with 12 processes

OpenMP

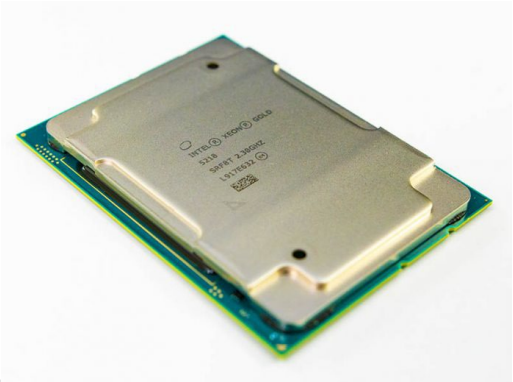
Test Name	6.2 12 threads	6.3 12 threads	63/62 Ratio
boston_lattice	306.38	280.52	0.92
godiva	1519.19	1452.16	0.96
manysurfaces	345.60	419.42	1.21
mode_n_air	225.00	229.79	1.02
mode_np_air	127.81	137.58	1.08
mode_npe_air	10.96	10.49	0.96
mode_p_air	579.87	517.37	0.89
mode_pe_air	13.18	13.63	1.03
pwr2d_whole	154.27	155.19	1.01
tally_void_f1	2440.68	2215.38	0.91
tally_void_f2	2426.97	2128.08	0.88
tally_void_f4	2149.25	2037.74	0.95
tally_void_f5	2492.31	2422.43	0.97
tally_void_fmesh	1155.08	1963.64	1.70
tally_void_ref	3145.63	2561.26	0.81
tally_fir	0.0241	0.0288	1.20
tally_kcode_fmesh	46.73	102.85	2.20
tally_pht	1689.39	1591.58	0.94
tally_phtvr	43.20	42.99	1.00
well_log	187.83	192.86	1.03
		Minimum	**0.81**
		Maximum	**2.20**
		Average	**1.08**

OpenMPI

Test Name	6.2 -np 12	6.3 -np 12	63/62 Ratio
boston_lattice	368.37	373.58	1.01
godiva	2731.31	2743.13	1.00
manysurfaces	303.45	377.14	1.24
mode_n_air	226.29	218.78	0.97
mode_np_air	121.47	125.32	1.03
mode_npe_air	10.21	9.95	0.97
mode_p_air	504.46	468.64	0.93
mode_pe_air	14.79	13.76	0.93
pwr2d_whole	158.37	162.71	1.03
tally_void_f1	2357.14	2262.86	0.96
tally_void_f2	2371.26	2329.41	0.98
tally_void_f4	2187.85	2175.82	0.99
tally_void_f5	3007.59	3046.15	1.01
tally_void_fmesh	2385.54	2289.02	0.96
tally_void_ref	3712.50	3666.67	0.99
tally_fir	0.02	0.0252	1.26
tally_kcode_fmesh	54.66	87.78	1.61
tally_pht	1557.30	1514.75	0.97
tally_phtvr	39.40	40.41	1.03
well_log	230.23	215.22	0.93
		Minimum	**0.93**
		Maximum	**1.61**
		Average	**1.04**

MCNP 6.2 and 6.3 Comparison: Windows-- Serial

- Windows 10
- Intel(R) Xeon(R) Gold 5218 CPU @ 2.30GHz
- 2 CPUs
  - 16 cores/CPU
  - 32 threads (hyperthreading on)
  - 2 NUMA nodes, one per CPU



	M histories per hour		63 / 62
Test Name	MCNP6.2	MCNP6.3	Ratio
boston_lattice	45.28	45.28	1.00
godiva	449.96	514.24	1.14
manysurfaces	46.15	49.32	1.07
mode_n_air	29.75	30.00	1.01
mode_np_air	14.06	15.13	1.08
mode_npe_air	1.21	1.13	0.94
mode_p_air	49.66	52.17	1.05
mode_pe_air	1.73	1.55	0.89
pwr2d_whole	20.01	20.01	1.00
tally_void_f1	283.46	281.25	0.99
tally_void_f2	285.71	281.25	0.98
tally_void_f4	255.32	250.00	0.98
tally_void_f5	464.52	469.57	1.01
tally_void_fmesh	352.94	342.86	0.97
tally_void_ref	586.96	600.00	1.02
tally_fir	0.0028	0.0031	1.11
tally_kcode_fmesh	12.20	12.11	0.99
tally_pht	105.88	118.87	1.12
tally_phtvr	5.14	5.07	0.99
well_log	29.03	27.48	0.95
		Minimum	0.89
		Maximum	1.14
		Average	1.01

Windows MCNP 6.2 and 6.3 Comparison – 12 threads

Test Name	6.2 12 threads	6.3 12 threads	63/62 Ratio
boston_lattice	405.63	411.43	1.01
godiva	2319.56	2495.41	1.08
manysurfaces	436.36	457.14	1.05
mode_n_air	237.36	278.71	1.17
mode_np_air	133.33	134.16	1.01
mode_npe_air	11.31	10.49	0.93
mode_p_air	464.52	482.68	1.04
mode_pe_air	14.78	14.33	0.97
pwr2d_whole	179.98	177.52	0.99
tally_void_f1	2541.18	2322.58	0.91
tally_void_f2	2541.18	2360.66	0.93
tally_void_f4	2261.78	2238.34	0.99
tally_void_f5	3840.00	3729.50	0.97
tally_void_fmesh	1728.00	2526.32	1.46
tally_void_ref	4563.38	4531.47	0.99
tally_fir		0.0256	
tally_kcode_fmesh	58.90	101.77	1.73
tally_pht	924.77	1064.79	1.15
tally_phtvr	46.96	44.31	0.94
well_log	193.72	236.07	1.22
		Minimum	0.91
		Maximum	1.73
		Average	1.08

FMESH improvements

Windows 6.3 Native – WSL-Ubuntu Comparison -- Serial

Test Name	M histories per hour: MCNP6.3 Native	MCNP6.3 WSL 1	MCNP6.3 WSL 2	WSL 1 / Native Ratio	WSL 2/ Native Ratio	WSL 2 / WSL 1 Ratio	Test Name
boston_lattice	45.28	48.00	48.32	1.06	1.07	1.01	boston_lattice
godiva	514.24	364.52	543.35	0.71	1.06	1.49	godiva
manysurfaces	49.32	44.17	49.66	0.90	1.01	1.12	manysurfaces
mode_n_air	30.00	30.51	31.30	1.02	1.04	1.03	mode_n_air
mode_np_air	15.13	15.93	15.65	1.05	1.03	0.98	mode_np_air
mode_npe_air	1.13	1.46	1.19	1.29	1.05	0.81	mode_npe_air
mode_p_air	52.17	70.59	52.17	1.35	1.00	0.74	mode_p_air
mode_pe_air	1.55	2.13	1.56	1.37	1.01	0.73	mode_pe_air
pwr2d_whole	20.01	21.41	20.98	1.07	1.05	0.98	pwr2d_whole
tally_void_f1	281.25	270.68	333.33	0.96	1.19	1.23	tally_void_f1
tally_void_f2	281.25	260.87	342.86	0.93	1.22	1.31	tally_void_f2
tally_void_f4	250.00	233.77	305.08	0.94	1.22	1.31	tally_void_f4
tally_void_f5	469.57	407.55	474.73	0.87	1.01	1.16	tally_void_f5
tally_void_fmesh	342.86	305.08	336.45	0.89	0.98	1.10	tally_void_fmesh
tally_void_ref	600.00	465.52	606.74	0.78	1.01	1.30	tally_void_ref
tally_fir	0.0031	0.003	0.0033	0.97	1.06	1.10	tally_fir
tally_kcode_fmesh	12.11	12.86	12.48	1.06	1.03	0.97	tally_kcode_fmesh
tally_pht	118.87	120.57	126.00	1.01	1.06	1.04	tally_pht
tally_phtvr	5.07	5.67	5.33	1.12	1.05	0.94	tally_phtvr
well_log	27.48	31.30	28.57	1.14	1.04	0.91	well_log
			Minimum	0.71	0.98	0.73	
			Maximum	1.37	1.22	1.49	
			Average	1.02	1.06	1.06	

Windows 6.3 Native – WSL-Ubuntu Comparison – 12 threads

	M histories per hour			WSL 1 / Native Ratio	WSL 2/ Native Ratio	WSL 2 / WSL 1 Ratio	
Test Name	MCNP6.3 Native	MCNP6.3 WSL 1	MCNP6.3 WSL 2				Test Name
boston_lattice	411.43	429.85	288.96	1.04	0.70	0.67	boston_lattice
godiva	2495.41	2541.29	2550.66	1.02	1.02	1.00	godiva
manysurfaces	457.14	423.53	445.36	0.93	0.97	1.05	manysurfaces
mode_n_air	278.71	295.89	265.03	1.06	0.95	0.90	mode_n_air
mode_np_air	134.16	157.66	137.58	1.18	1.03	0.87	mode_np_air
mode_npe_air	10.49	13.58	10.43	1.30	1.00	0.77	mode_npe_air
mode_p_air	482.68	691.20	438.58	1.43	0.91	0.63	mode_p_air
mode_pe_air	14.33	18.85	13.70	1.32	0.96	0.73	mode_pe_air
pwr2d_whole	177.52	190.56	170.51	1.07	0.96	0.89	pwr2d_whole
tally_void_f1	2322.58	2571.43	2716.98	1.11	1.17	1.06	tally_void_f1
tally_void_f2	2360.66	2618.18	2716.98	1.11	1.15	1.04	tally_void_f2
tally_void_f4	2238.34	2285.71	2526.32	1.02	1.13	1.11	tally_void_f4
tally_void_f5	3729.50	3676.60	3600.00	0.99	0.97	0.98	tally_void_f5
tally_void_fmesh	2526.32	1494.81	1687.50	0.59	0.67	1.13	tally_void_fmesh
tally_void_ref	4531.47	4378.38	4291.39	0.97	0.95	0.98	tally_void_ref
tally_fir	0.0256	0.0077	0.0288	0.30	1.13	3.74	tally_fir
tally_kcode_fmesh	101.77	61.70	106.22	0.61	1.04	1.72	tally_kcode_fmesh
tally_pht	1064.79	1913.92	1053.66	1.80	0.99	0.55	tally_pht
tally_phtvr	44.31	52.68	46.45	1.19	1.05	0.88	tally_phtvr
well_log	236.07	263.41	217.09	1.12	0.92	0.82	well_log
			Minimum	0.30	0.67	0.55	
			Maximum	1.80	1.17	3.74	
			Average	1.06	0.98	1.08	

Los Alamos NATIONAL LABORATORY

MCNP MONTE CARLO N-PARTICLE

Conclusions

- In general, there are no the performance differences between MCNP6.2 and MCNP6.3
- Significant performance improvements in MCNP6.3 were made for
  - Unstructured mesh
  - FMESH tallies
  - ACT card DG = line option
- There are no significant performance differences between using the native Windows, WSL 1, or WSL 2 environments on Windows computers.

Breaking News Courtesy of Tim Burke

Here are the results from grace and snow that I got. Grace is 1 chip, 72 cores. Snow node is 2 chips, 18 cores each.
The Grace build used GCC 12.3 and MPI 4.1.5 – 3.1.6 fails on those nodes with newer RHEL (It's actually RHEL 9)
I built the same devel branch on snow using GCC 11.2 and OpenMPI 4.1.1.

……

Model	CTS-1	Grace	Grace/CTS-1 Speedup
Godiva	8524.36	27732.71	3.25
Zeus	1040.76	4540.25	4.36
BEAVRS, no DBRC	220.29	857.71	3.89

There was a non-negligible amount of variance in the performance as the number of histories/cycle changed on each machine.

For example, using 100K or 3M histories/cycle on BEAVRS saw the performance drop to ~550 M/hr.
For BEAVRS I chose a number that ran well on Grace without doing a search for CTS-1, so that node's performance may not be as optimal.

Of note, it looks like one half of a grace Superchip is 250 W. A whole chip is 2 CPUs and up to 960 GB memory for 500 W
And the CPUs on one node of snow is 120 x 2 = 240 W.

So this is a rough 3-4x improvement in raw performance AND in performance per watt. Neat!