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Title: QUADRENNIAL MCNP TIMING STUDY

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ABSTRACT

The Los Alamos National Laboratory Monte Carlo N-Particle radiation transport code, MCNP[1], is widely used around the world for many radiation protection and shielding applications. As a well-known standard it is also an excellent vehicle for assessing the relative performance of scientific computing platforms.

Every three-to-four years a new version of MCNP™ is released internationally by the Radiation Safety Information Computational Center (RSICC) in Oak Ridge, Tennessee. For each of the past few releases, we have also done a timing study to assess the progress of scientific computing platforms and software. These quadrennial timing studies are valuable to the radiation protection and shielding community because: (a.) they are performed by a recognized scientific team, not a computer vendor, (b.) they use an internationally recognized code for radiation protection and shielding calculations, (c.) they are eminently reproducible since the code and the test problems are internationally distributed.

Further, if one has a computer platform, operating system, or compiler not presented in our results, its performance is directly comparable to the ones we report because it can use the same code, data, and test problems as we used.

Our results, using a single processor per platform, indicate that hardware advances during the past three years have improved performance by less than a factor of two and software improvements have had a marginal effect on performance. The most significant impacts on performance have resulted from developments in multiprocessing and multitasking. The other most significant advance in the last three years has been the accelerated improvements in personal computers. In the last timing study[3], the tested personal computer was approximately a factor of four slower that the fastest machine tested, a DEC Alphastation 500. In the present study, the fastest PC tested was less than a factor of two slower than the fastest platform, which is a Compaq (previously DEC) Alpha XP1000.

I. INTRODUCTION

Following in the traditions of previous releases[2,3], the most current release of MCNP, version 4C[1], has been executed on an array of computing platforms. The machines involved ranged from desktop workstations to supercomputers capable of massive parallel processing. For the purposes of performance comparisons between different platforms and consistency with previous studies, all test cases were conducted with a single processor on each platform. The foundation for this analysis is a 29 problem test set which was developed for coverage analysis of a previous release of MCNP.[4] There have been a few modifications to this test suite for the most recent release of the code.

MCNP has become an international standard for a wide spectrum of radiation transport applications, including radiation shielding, health physics, medical physics, nuclear criticality safety, nuclear safeguards, nuclear well-logging, fission and fusion reactor design,

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accelerator target design, detector design and analysis, decontamination and decommissioning, and waste storage and disposal.

The overall development philosophy of MCNP revolves around the edicts of quality, value, and features. MCNP4C contains ten principal new features since version 4B,[5] including macrobodies, superimposed meshes for variance reduction, perturbation enhancements, electron physics enhancements, unresolved resonance probability tables, new ENDF/B-VI sampling capabilities, delayed neutrons, alpha eigenvalue search, parallelization enhancements, and upgraded PC capabilities. The portability of the code is demonstrated by the support of nine computer systems. A comprehensive discussion and review of the new advances in version 4C of the code is found in a companion paper in this conference.[6]

II. IMPORTANT CONSIDERATIONS RELEVANT TO PERFORMANCE COMPARISONS

The timing study for the recent release of MCNP4C has been carried out on all the nine supported platforms. The personal computers were evaluated with two processors of different capabilities. In order to compare the performance for a given computer code and to understand the different metrics used, it is instructive to identify the major important considerations that influence the performance. These considerations are comprised of a complicated function of many variables and may include:

- Computer architecture, either vector-based or cache-based. Many cache-based systems have RISC (reduced instruction set computer) architectures.
- Processor clock speed.
- Number of floating point operations per clock cycle. This is important for Monte Carlo analysis since particle transport involves floating point intensive operations.
- Number of instructions issued per clock cycle.
- The memory band width, which is associated with the bus speed.
- The size of cache (for a cache-based system).
- The size of the Random Access Memory (RAM). In order to maximize performance, it is preferable to have the code reside in memory and to minimize access to the hard disks.
- The operating system (type and version).
- The Fortran Compiler (type and version).
- Processor chip manufacturer.
- 64-bit verses 32-bit architecture.

It is important to emphasis that a single metric, such as clock speed may be misleading in representing the system performance. One illustration of this is the comparison of the Cray T90 and the SGI Origin 2000. The Cray is a vector-based machine with a parallel vector processor (PVP). By contrast, the SGI Origin 2000 is a cache-based system with a RISC architecture and a symmetric multiprocessor (SMP). Codes whose construction has been vectorized will generally perform better on the Cray than on the SGI. In this study, we evaluated MCNP4C on the Cray T90 (454 MHz) and on the SGI Origin 2000 (250 MHz). As will be demonstrated in the results below, the SGI shows superior performance compared with the Cray. This is due to the fact that MCNP is not a vectorized code.

With the exception of the Cray, all other systems evaluated in this study are cache-based systems, and of these, all but the personal computers have a RISC architecture.

III. RESULTS OF TIMING STUDY

We have evaluated the computer clock time for the following computer systems: the Compaq (previously DEC) Alpha XP1000, PC Digital Visual Fortran (Intel Pentium II and III), and PC Lahey Fortran (Intel Pentium II and III), SGI Origin 2000, Sun Ultra 80, PC Linux, HP 9000-735, Cray T90, IBM RS/6000-590. The computer clock speeds of the individual processors range from 66 MHz to 600 MHz. As discussed in the previous section, the clock speed is only one of many variables that influence performance. Amongst these platforms, the fastest "state-of-the-art" computers include the Compaq Alpha XP1000, PC Intel Pentium III, SGI Origin 2000, and the Sun Ultra 80.

Table I provides information on the computer platform description, clock speed, operating system, and Fortran compiler version.

Table I.

Computer System Description

Computer Platform	Clock Speed	Operating System	Fortran Compiler
Compaq Alpha XP1000	500 MHz	Version 5.0 Alpha	F77 Version 5.3-915
PC / Intel Pentium III	600 MHz	Windows NT 4.0	Digital Visual Fortran (DVF) F90 v 6.0
PC / Intel Pentium III	600 MHz	Windows NT 4.0	Lahey Fortran 95 (LF 95) v 5.50h
SGI Origin 2000	250 MHz	IRIX 6.4	MIPS Pro F77 7.2.1
Sun Ultra 80	450 MHz	Solaris 8	F77 5.0
PC / Intel Pentium II	450 MHz	Windows NT 4.0	Digital Visual Fortran (DVF) F90 v 6.0
PC / Intel Pentium II	450 MHz	Windows NT 4.0	Lahey Fortran 95 (LF 95) v 5.50h
PC / AMD K6-2 / Linux	450 MHz	Linux / Redhat 6.0	GNU G77 0.5.25
HP / 9000 - 735	125 MHz	HP UX 9000 B.10.20	F77 B.10.20
Cray T90	454 MHz	Unicos	CFT77 6.0.4.21
IBM RS / 6000 - 590	66 MHz	AIX 4.1.5	XLF 3.2.5.0

Table II shows the running times of the 29-problem regression test suite for MCNP4C on each of the computer platforms listed in the above table. The execution of these problems was carried out in a sequential mode on a single processor. The times reported are the particle transport times in CPU minutes, and do not include the problem setup, cross section data retrieval, or input/output times. For many of the test problems, the setup time is comparable to that of the particle transport time due to the low number of particle histories associated with the execution of these test problems. Increasing the number of histories will result in an increase in particle transport time that scales approximately with the increase in the number of histories. The setup and input/output times will not significantly increase.

The Cray and Compaq Alpha are 64-bit machines and all results on these machines represent a 64-bit compilation. With the exception of the SGI, the executables on all remaining systems represent 32-bit compilations. The results in Table II for the SGI correspond to a 64-bit compilation of the code. The timing results for this machine were also obtained for a 32-bit compilation, yielding a negligible difference in the performance numbers generated.

The results in Table II show that the fastest system tested in this study is the Compaq Alpha XP1000. This is using a new Alpha 21264 processor, which is a full 64-bit processor, based on advanced RISC technology. This system has a 4 MB L2 cache, delivers 2.6 GB/second bandwidth, dual independent 32/64 bit PCI buses, and an integrated Wide-Ultra SCSI disk subsystem. It should be noted that the fastest system tested in the 1997 study was the DEC Alphastation 500, which is a predecessor to the XP1000, and the fastest system tested in the 1993 study was the HP 9000-735.[2,3]

In the current study, the next fastest machine is the PC with the 600 MHz Pentium III processor. The performance on both PC Fortran compilers, Digital Visual Fortran (DVF) F90 and Lahey Fortran F95, was less than a factor of two slower than the Compaq Alpha XP1000. The DVF compiler was approximately 15% faster than the Lahey Fortran compiler for the same computer system. The next fastest machine was the SGI Origin 2000, which was approximately a factor of two slower than the Compaq Alpha XP1000. Following this are the Sun Ultra 80, the PC Intel Pentium II systems, and the PC Linux systems all having 450 MHz clock speeds. Of these, the PC/Linux system with the AMD chip and running the GNU g77 compiler is the slowest. Other compilers for the Linux operating system, such as the Portland compiler, may run faster. The next fastest platform is the HP 9000-735, which is approximately seven times slower than the Compaq Alpha XP1000, but was the fastest platform in the 1993 study.[2] Finally, the Cray T90 runs MCNP4C approximately eight time slower than the Compaq Alpha XP1000, and the IBM RS/6000-590 runs almost a factor of ten slower than the Compaq Alpha XP1000.

Of particular significance is the fact that, in the 1997 study, the tested PC was approximately a factor of four slower than the fastest tested machine, the DEC Alphastation 500; whereas, in the current study, the PC Pentium III was less than a factor of two slower than the fastest machine, the XP1000. This is due to the significant advances in the designs and performance of personal computers in the last three years, as well as to enhancements in the 4C version of MCNP for personal computer platforms which take advantage of the developing technologies.

IV. SUMMARY

A timing study has been performed on the recently released version 4C of the MCNP code on all the nine supported systems. The results show that the fastest machine is the Compaq Alpha XP1000, whose predecessor is the DEC Alphastation 500, the fastest machine in the 1997 timing study for MCNP version 4B. The performance comparison between these two machines for MCNP4C is within a factor of two. The most significant advance in computer hardware during the last three years is in the improvements in the performance of personal computers. The other advances of interest have been in the field of parallel processing. MCNP will continue to develop to further take advantage of the new capabilities introduced in the developing computer technologies, both for personal computers and for parallel processing.

REFERENCES

1. J. F. Briesmeister, Ed., "MCNP – A General Monte Carlo N-Particle Transport Code, Version 4C," LA – 13709-M (April 2000).

2. J. S. Hendricks, R. C. Brockhoff, "Comparison of Scientific Computing Platforms for MCNP4A Monte Carlo Calculations," *Nucl. Sci. Eng.*, **116**, 269-277 (1994)

3. H. E. McLaughlin, J. S. Hendricks, "Performance of Scientific Computing Platforms with MCNP4B," *Nucl Sci. Eng.*, **129**, 311-319, (1998).

4. R. C. Brockhoff, J. S. Hendricks, "A New MCNP Test Set," LA-12839, Los Alamos National Laboratory (September 1994).

5. J. F. Briesmeister, Ed., "MCNP – A General Monte Carlo N-Particle Transport Code, Version 4B," LA – 12625-M (May 1997).

6. J. S. Hendricks, "Advances in MCNP4C," Radiation Protection for our National Priorities, Spokane, Washington, September 17-21, 2000, LA-UR-00-2643, Los Alamos National Laboratory (2000).

TABLE II.

Particle Transport Times for MCNP4C Using MCNP4C Test Set

CPU Minutes

Test Problem	Compaq Alpha XP1000 500 MHz	PC / NT DVF 600 MHz	PC / NT LF 95 600 MHz	SGI Origin 2000 250 MHz	Sun Ultra 80 450 MHz	PC / NT DVF 450 MHz	PC / NT LF 95 450 MHz	PC / Linux G77 450 MHz	HP 9000 -735 125 MHz	Cray T90 454 MHz	IBM RS / 6000-590 66 MHz
01	0.01	0.01	0.02	0.02	0.02	0.03	0.03	0.06	0.06	0.06	0.09
02	0.02	0.03	0.03	0.04	0.05	0.06	0.06	0.12	0.15	0.13	0.18
03	0.02	0.03	0.03	0.04	0.05	0.05	0.05	0.11	0.16	0.17	0.19
04	0.03	0.06	0.06	0.06	0.08	0.09	0.09	0.19	0.24	0.23	0.31
05	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.04	0.04	0.05	0.06
06	0.01	0.02	0.02	0.02	0.03	0.03	0.05	0.07	0.08	0.09	0.11
07	0.04	0.05	0.06	0.06	0.07	0.08	0.09	0.20	0.21	0.26	0.32
08	< 0.01	<0.01	<0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.02
09	0.02	0.02	0.03	0.03	0.04	0.06	0.05	0.10	0.10	0.11	0.15
10	0.01	0.02	0.03	0.03	0.04	0.04	0.05	0.09	0.10	0.10	0.15
11	0.04	0.07	0.09	0.08	0.10	0.11	0.13	0.26	0.27	0.35	0.39
12	0.06	0.10	0.12	0.12	0.18	0.16	0.19	0.42	0.45	0.53	0.70
13	0.01	0.02	0.02	0.02	0.02	0.03	0.03	0.05	0.07	0.10	0.11
14	0.01	0.02	0.02	0.03	0.03	0.03	0.04	0.07	0.08	0.11	0.12
15	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.04	0.04	0.05	0.05
16	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.03	0.03	0.04	0.05
17	0.02	0.03	0.04	0.04	0.05	0.07	0.06	0.12	0.16	0.21	0.21
18	0.05	0.08	0.12	0.11	0.12	0.12	0.17	0.28	0.35	0.45	0.48
19	0.02	0.04	0.04	0.05	0.07	0.08	0.07	0.16	0.25	0.21	0.27
20	0.04	0.08	0.09	0.08	0.13	0.11	0.12	0.28	0.35	0.35	0.48
21	0.06	0.07	0.09	0.10	0.11	0.12	0.15	0.29	0.33	0.38	0.45
22	0.01	0.01	0.01	0.01	0.02	0.01	0.03	0.04	0.05	0.06	0.07
23	0.03	0.07	0.07	0.07	0.11	0.09	0.10	0.22	0.35	0.29	0.39
24	0.02	0.03	0.03	0.04	0.04	0.05	0.06	0.11	0.12	0.16	0.19
25	0.03	0.04	0.05	0.06	0.06	0.07	0.09	0.16	0.17	0.23	0.27
26	0.02	0.03	0.03	0.03	0.04	0.06	0.05	0.10	0.11	0.12	0.16
27	0.01	0.02	0.02	0.02	0.03	0.03	0.03	0.07	0.07	0.09	0.11
28	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.04	0.04	0.04	0.06
29	0.05	0.08	0.09	0.11	0.15	0.12	0.13	0.31	0.48	0.50	0.60
Total	**0.68**	**1.07**	**1.25**	**1.33**	**1.71**	**1.77**	**2.01**	**4.04**	**4.93**	**5.49**	**6.74**