TITLE RECENT MCNP DEVELOPMENTS

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Recent MCNP Developments

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Abstract

We report here both the status and recent developments in the MCNP Monte Carlo radiation transport computer code and also two items of more general interest to computational physics: the accuracy of modern physics computer codes and the performance of scientific workstations.

1 MCNP Introduction

MCNP is a Monte Carlo continuous-energy, three-dimensional neutron-photon-electron radiation transport computer code used in many industries, including nuclear well logging, medical imaging, and nuclear reactors. A general overview of MCNP was presented at the IEEE 1989 Nuclear Science Symposium[1]. Here we focus upon (1) a number of recent significant advances and new directions for MCNP; (2) the MCNP benchmark project that also provides insight into the reliability of modern computer codes and data libraries; and (3) a new timing study measuring the performance of MCNP on several computing platforms.

MCNP version 4 was released internationally in March 1991, featuring for the first time electron transport, a thick-target bremsstrahlung model, multitasking, pulse-height tallies, and other features. Several new Monte Carlo research programs are underway relating to MCNP and many new features are being prepared for the upcoming MCNP4A version of the code.

A program to benchmark the code against a wide variety of experimental measurements has reached a major milestone. Not only does this project document the accuracy of MCNP for neutron and photon transport problems, but it also provides insight into how well modern physics computer codes can model a variety of experiments.

As part of the evolution from being a Cray code to a UNIX code supported on many computer platforms, a timing study was made comparing performance of Sun, IBM, and HP workstations to the Cray. The results are reported here for the first time.

2 MCNP Overview and Status

MCNP is a general purpose Monte Carlo code for calculating the time-dependent continuous-energy transport of neutrons, photons, and/or electrons in three-dimensional geometries. Both fixed source and k_{eff} criticality problems can be solved and a number of output tally options are available. Data representations either can be fully or partially continuous or multigroup. The code is rich in variance reduction techniques that improve the efficiency of difficult calculations. The documentation for MCNP is a 600-page manual[2] describing the Monte Carlo theory, geometry, physics, cross sections, variance reduction techniques, tallies, errors, input, and output.

MCNP is used for many applications: reactor design (both fission and fusion), nuclear criticality safety, radiation shielding, nuclear safeguards, detector design and analysis, nuclear well logging, personnel dosimetry and health physics, accelerator target design, medical physics and radiotherapy, aerospace applications, defense applications, radiography, waste disposal, and decontamination and decommissioning. Recent major applications at Los Alamos include the space exploration initiative, general criticality safety, strategic nuclear materials safeguards, accelerator transmutation of nuclear waste, and safety analysis for the DOE New Production Reactor. Facilities designed with or having safety analysis performed by MCNP include the Dual Axis Radiographic Hydro Test facility (DARHT), the target area for the Manuel Lujan, Jr., Neutron Scattering Center (LANSCE), and the Materials Processing Laboratory radiological dose reduction studies.

MCNP is distributed for Los Alamos by the Radiation Shielding and Information Center (RSIC) in Oak Ridge, Tennessee. They receive requests for the code from about 50 institutions per year. MCNP also is distributed by the NEA Data Bank in France and can be accessed by anyone with an account on the Los Alamos Integrated Computing Network. We estimate that there are hundreds, perhaps more than a thousand, active users around the world at perhaps one hundred installations.

The Monte Carlo method was developed at Los Alamos during the Manhattan Project in the early 1940s. The current MCNP code is the heir to those early efforts. More than 350 person years have been invested into the re-

search, development, programming, documentation, and data bases for MCNP. The first multipurpose code version was written in 1963. In the mid-70's, neutron and photon codes were merged to form MCNP, which has undergone major upgrades approximately every two to three years since. MCNP3 was released in 1983 and rewritten in standard Fortran. MCNP3A was released in 1985 and featured a very flexible generalized source. MCNP3B was released in 1988, featuring a repeated structures and/or lattice capability, a multigroup option, and tally output plotting.

MCNP4 was released in July 1990 at Los Alamos and in March 1991 to the Reactor Shielding and Information Center at Oak Ridge (version MCNP4.2). There are hundreds of minor improvements in addition to the following major new features:

- A continuous-energy electron transport package based on the Sandia National Laboratories Integrated Tiger Series (ITS)[3] has been incorporated into MCNP along with the associated data base.
- A thick-target bremsstrahlung approximation has been incorporated to model electron-induced photon production using the ITS electron data. The model includes much of the electron physics for photon generation at only a fraction of the cost of the fully-continuous-energy electron treatment.
- Shared memory multitasking has been added for multitasking workstations and the Cray multiprocessor mainframes. The clock turnaround for multitasked problems is reduced by approximately the number of processors used in the calculation.
- A pulse-height tally model is now available that records the energy deposited in a cell by each source particle and its secondary particles. Unlike other MCNP tallies, the pulse height tally models microscopic rather than macroscopic events.
- The criticality eigenvalue source can now use the full generality of other MCNP sources for the initial conditions in k_{eff} problems.
- MCNP can be interrupted interactively to request plots of tally quantities.
- Next-event estimators such as point detectors and the DXTRAN variance reduction scheme can now be used with $S(\alpha, \beta)$ thermal scattering.[4,5]
- MCNP4 is the first MCNP version designed specifically for UNIX systems and has data paths built in and shell scripts distributed with the code, along with answer sets for specific systems.

3 MCNP4A

The next version of MCNP will be MCNP4A, scheduled for release in late 1992 or early 1993. The code will continue to evolve more towards a Unix workstation-based code. We believe that if massively parallel systems become widely available, they will have shared memory and be available with Unix and standard Fortran 77. Even workstations will become highly parallel. In the meantime, the current generation of workstations will become increasingly important as their performance approaches that of supercomputers. As shown in the timing studies presented later, some workstations already approach the Cray mainframes in performance.

Significant new features under active development for incorporation into MCNP4A are:

- ENDF/B-VI physics. The recent ENDF/B-VI data libraries include a number of new formats and formalisms such as correlated energy-angle scattering;
- Photons to 1 GeV. Although the MCNP4 electron/photon physics is based upon the Integrated Tiger Series, the present photon data only goes up to 100 MeV. MCNP is being given the capability to read multiple data sets with physics models appropriate to ranges up to 1 GeV;
- Improvements in the electron-photon transport package, including charge deposition tallies and variable electron substep sizes;
- A quasi-deterministic weight window generator developed [6,7] to more efficiently automatically estimate an optimum importance function for variance reduction than does the present scheme[8];
- The DXANG angle bias method[9] for particle collisions provides a numerically stable means of directionally biasing particles emerging from collisions;
- Expansion of the tallying capabilities for problems with lattices and repeated structures to permit tallying isolated components that are repeated;
- Periodic and white boundary conditions have been added;
- MCNP4A will write out history tapes for postprocessing either by the SABRINA color graphics code[10] to illustrate particle tracks or by the LAHET (high energy transport) code[11];
- The source model will include intrinsic radiation sources[12] to model radioactive decay.

Other major new features that we would like to put into MCNP if time and resources permit are:

- Upgrading the Integrated Tiger Series physics to ITS version 3.0, and incorporation of EGS4 [13] physics as appropriate;

- Probability table treatment for the unresolved range neutron cross section data;
- A generalized perturbation treatment.

A number of research projects are under way which will certainly have long-range effects upon MCNP, though perhaps not MCNP4A. These programs are funded by computer companies, oil services companies, the Department of Energy and some competitive Los Alamos National Laboratory discretionary research funding. They are:

- Variance-of-variance. A modified version of MCNP is available that scores the variance of the tally variance and produces a history score probability density function to provide more information on how reliable the MCNP estimated answers are.[14]
- Dataflow. A stripped-down version of MCNP has been written in the Id dataflow language, which is an advanced computer language designed for massively parallel MIMD (Multiple Instruction Multiple Data) computers.
- Oil and gas well logging (proprietary projects).
- Criticality problem eigenfunction stabilization. Although Monte Carlo can do an excellent job estimating eigenvalues (k_{eff}) of critical systems, the principal eigenfunction, such as the flux distribution across a reactor core, is sometimes estimated quite poorly with misleading error estimations.
- Variance reduction for collective multiparticle events. Some Monte Carlo estimates, for example, the pulse height tally, require detailed simulation of microscopic events. Current variance reduction techniques are correct for tallies determined by the behavior of individual particles, but not applicable when the tally is determined by the behavior of a collection of particles. The modeling of collective (or non-Boltzmann) transport is incompatible with normal variance reduction techniques, and new variance reduction methods must be developed.

MCNP is a sponsor- and user-driven computer code. Our sponsors determine what they want us to add to the code, and user feedback leads to many improvements. New features are incorporated into the code only after peer review, an extensive testing program, and residency in "patched versions," where algorithm robustness and sustained user interest and satisfaction must be demonstrated.

The large number of Monte Carlo research projects and MCNP4A development projects underway testifies to the continued vitality of the MCNP program.

4 MCNP Benchmarking

A major milestone has been reached in an ongoing program to formally benchmark MCNP. Two publications have

just been released comparing MCNP calculations with a wide variety of analytic and photon benchmarks[15] and with three major classes of neutron experimental measurements[16]. These benchmarks not only serve to validate MCNP, but also indicate the high degree of reliability of modern computational methods and data.

In the first publication, LA-12196, analytic and photon benchmarks are considered. As would be expected, MCNP agrees with analytic problems to within the statistical uncertainty. Three families of photon experiments were also calculated: a gamma-ray skyshine experiment, a ^{60}Co air-over-ground experiment, and thermoluminescent dosimeter (TLD) experiments. These problems were deep penetration and streaming problems, and all required elaborate variance reduction. In all cases MCNP did well, agreeing to within statistical and measured uncertainties for all but the deepest penetrations. For penetrations on the order of ten mean free paths deep, MCNP usually was within a factor of two of the measurement, which often times was of questionable accuracy.

In the second publication, LA-12212, three families of neutron benchmarks are compared: the Livermore pulsed sphere measurements, the Oak Ridge fusion shielding benchmarks, and, finally, nine critical assemblies. The critical assemblies ranged from simple Godiva and Jezebel spheres to complicated arrays, and all converged sufficiently near $k_{eff} = 1$.

The Oak Ridge fusion shielding benchmarks involved streaming, deep penetration, and generation of neutron-induced photons. Fourteen-MeV neutrons were emitted isotropically and streamed down an iron pipe embedded in concrete before penetrating shields of 30.5 cm iron, or 46 cm iron and 10 cm of borated polyethylene. Neutrons and secondary photons then were measured at points on- and off-axis beyond the shield. Considering the deep penetration of up to 25 mean free paths, both neutron and photon results were excellent. Throughout the energy range, detailed-spectral results were always within a factor of two and integral results (the total flux at off-axis detectors) were never more than 25% off from the measurement. For shallower penetrations the calculations agreed with measurements within statistics.

The Livermore pulsed spheres used a 14-MeV neutron source and measure penetration of a wide variety of materials of various thicknesses at several angles. The results for 28 spheres indicate that the Monte Carlo results agree with the measurements except when the cross section data are poorly known. In the worst case, a liquid nitrogen sphere 7.7 mean free paths thick, MCNP differed from the experiment by 29% in the worst energy range and by 7% overall. By switching from ENDF/B-V cross sections to ENDF/B-VI data, the disagreement lessened to 13% and 3%, respectively.

From these benchmark calculations we conclude that modern computational methods, such as MCNP, are capable of accurately modeling neutron and photon physics in the applicable energy ranges to essentially the accuracy

of the cross section data. For shallow penetrations we have full confidence in the calculational results. For deeper penetrations where small uncertainties in the physics data can build up to systematic deviations from measurement, we observe that even at 10 to 25 mean free paths the calculations are usually within a factor of two of measurements.

The two benchmark reports are available free to anyone contacting the authors. The E-mail address is MCNP@LANL.GOV.

These benchmarks are part of an ongoing project[17,18]. A cooperative program being carried out at General Electric, San Jose, consists of MCNP light water reactor benchmark problems[19,20]. A subsequent phase focusing on electron problems is planned.

5 Timing Study

We have recently completed a timing study comparing the performance of MCNP on the Cray-YMP264, Cray-XMP416, Sun Sparc 1, Sun Sparc 2, IBM RS/6000-550, and HP 9000/730. This paper is the first public disclosure of the results of this particular timing study, which has the following characteristics:

- It is limited to MCNP. We believe the results do not extrapolate to other computer codes. In particular, MCNP performs well on workstations relative to the Cray mainframes because MCNP does not vectorize well. For codes that vectorize, the Cray should perform much better than the workstations.
- The results we report are for the hardware and software available to us October 1991. The Fortran compilers used were the Sun 1.4, HP 8.05, IBM XLF2.2, and Cray CFT77 version 5.0.0.7 (UNICOS). Advances in both hardware and software, particularly compilers, will inevitably make our reported results obsolete.
- This timing study used a real production-version physics code.
- The problems used are the 25 MCNP test set problems available from RSIC. Our timing comparison is not limited to a single "typical" test problem.
- The results are reproducible. We report the MCNP performance (particle histories per minute) for each system. Anyone with a similar workstation and compiler can get the same test problem set and the same MCNP4.2 code from RSIC and replicate our results.

A typical set of performance data for the twenty-five MCNP test problems on the six machines is presented in Table 1. These data are normalized to the Cray YMP in Table 2, and to the IBM RS/6000-550 in Table 3. The average performance for the six systems relative to the YMP and based upon running the 25-problem set on each machine 3 - 7 times can be summarized as YMP = 100%.

XMP = 86%, HP-730 = 91%, IBM-550 = 60%, Sun Sparc 1 = 12% and Sun Sparc 2 = 24%.

The highest level of optimization for each compiler was used to the best of our ability. All runs were done in 64-bit mode, although the workstations used 32-bit cross-section data. Timing results were obtained through the use of MCNP routines that return elapsed cpu plus system time as opposed to wallclock time or time in cycles. The performance for each problem on each machine rarely varied more than a few percent from trial to trial and was always within 10%.

We were surprised to see how strongly problem dependent our results were. For example, the IBM-550 consistently ranges from about 50% to 80% of the performance of the Cray YMP depending upon the problem. Therefore, we believe that studies comparing performance based upon a single "typical" problem can be very misleading.

We also found that performance was very sensitive to the compiler version used and the optimization level chosen. The performance of particular problems on the same machine with different optimization levels varied significantly. For example, on the Cray XMP problem 6 was the best performer with one optimization level and problem 11 was the best performer with another optimization level. On some machines we observed performance differences as much as 50% for different compilers and optimization levels.

We wish to repeat the caveats of one of our earlier published timing comparisons[21]. The performance of scientific workstation hardware and software is improving so rapidly that most measures are outdated by the time they are published. These performance figures give a relative comparison at one instant in time and are presented for information only.

One conclusion is clear from these timing studies. Scientific workstations today can approach the performance available only from mainframes a few years ago.

6 Summary

MCNP is a widely used and actively developed Monte Carlo radiation transport code. Many important features have recently been added and more are under development. Benchmark studies not only indicate that MCNP is accurate, but also that modern computer codes can give answers basically as accurate as the physics data that goes in them. Even deep penetration problems can be correct to within a factor of two after 10 to 25 mean free paths of penetration. And finally, Monte Carlo calculations, once thought to be too expensive to run routinely, can now be run effectively on desktop computers which compete with the supercomputers of yesteryear.

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TABLE 1

MCNP PERFORMANCE (particle histories per minute)

Test Problem	YMP	XMP	Sun Sparc1	Sun Sparc2	IBM-550	HP-730
1.	7.1224E+4	5.9703E+4	7.3082E+3	1.5121E+4	3.7221E+4	5.8824E+4
2.	2.2188E+4	1.8704E+4	2.0580E+3	4.4248E+3	1.2058E+4	1.8270E+4
3.	1.8622E+4	1.6237E+4	2.6062E+3	5.9488E+3	1.3342E+4	2.0783E+4
4.	9.4285E+3	8.0183E+3	7.9256E+2	1.7986E+3	4.9727E+3	7.1908E+3
5.	2.0661E+3	1.7499E+3	1.5492E+2	3.6364E+2	1.0844E+3	1.5460E+3
6.	5.5836E+4	4.6859E+4	5.6022E+3	1.2010E+4	2.9499E+4	4.8780E+4
7.	1.8000E+4	1.5549E+4	2.2759E+3	4.8591E+3	1.1050E+4	1.8416E+4
8.	5.2182E+3	4.2544E+3	4.4183E+2	1.0714E+3	2.6923E+3	3.3281E+3
9.	3.4869E+4	3.0248E+4	5.3109E+3	1.1051E+4	2.5285E+4	4.0911E+4
10.	3.6352E+3	3.0767E+3	3.0525E+2	6.8259E+2	1.8029E+3	2.5751E+3
11.	7.9454E+3	7.3203E+3	9.3985E+2	2.1572E+3	5.8575E+3	8.9109E+3
12.	4.0817E+3	3.5007E+3	3.7959E+2	8.3577E+2	2.1544E+3	3.0136E+3
13.	2.6404E+4	2.3082E+4	3.6643E+3	8.3091E+3	2.1164E+4	3.4904E+4
14.	2.6560E+4	2.3252E+4	5.2306E+3	1.0648E+4	2.1490E+4	3.5993E+4
15.	2.1260E+4	1.8687E+4	3.2310E+3	6.4034E+3	1.3319E+4	2.4641E+4
16.	1.2064E+4	1.0332E+4	1.8328E+3	3.6729E+3	7.7781E+3	1.2976E+4
17.	1.4883E+4	1.2558E+4	1.6950E+3	3.6137E+3	9.3520E+3	1.3350E+4
18.	1.3017E+3	1.2104E+3	2.2095E+2	4.7372E+2	1.0808E+3	1.8551E+3
19.	5.3358E+3	4.6138E+3	6.6262E+2	1.4055E+3	2.6490E+3	4.4280E+3
20.	2.1523E+4	1.7562E+4	1.7580E+3	4.3343E+3	1.2690E+4	1.2277E+4
21.	3.1801E+4	2.7927E+4	3.9481E+3	7.9734E+3	1.9036E+4	2.8289E+4
22.	3.8328E+3	3.3800E+3	5.3422E+2	1.1577E+3	2.4343E+3	3.6923E+3
23.	5.6890E+3	4.6908E+3	4.6671E+2	1.1478E+3	3.2189E+3	3.4572E+3
24.	1.8468E+3	1.6629E+3	2.9949E+2	6.3766E+2	1.3169E+3	2.0979E+3
25.	3.7108E+4	3.2402E+4	6.0809E+3	1.2409E+4	2.6240E+4	4.4375E+4

TABLE 2

MCNP PERFORMANCE NORMALIZED TO CRAY-YMP

	YMP	XMP	Sun Sparc1	Sun Sparc2	IBM-550	HP-730
1.	100	84	10	21	52	83
2.	100	84	9	20	54	82
3.	100	87	14	32	72	112
4.	100	85	8	19	53	76
5.	100	85	7	18	52	75
6.	100	84	10	22	53	87
7.	100	86	13	27	61	102
8.	100	82	8	21	52	64
9.	100	87	15	32	73	117
10.	100	85	8	19	50	71
11.	100	92	12	27	74	112
12.	100	86	9	20	53	74
13.	100	87	14	31	80	132
14.	100	88	20	40	81	136
15.	100	88	15	30	63	116
16.	100	86	15	30	64	108
17.	100	84	11	24	63	90
18.	100	93	17	36	83	143
19.	100	86	12	25	50	83
20.	100	82	8	20	59	57
21.	100	88	12	25	60	89
22.	100	88	14	30	64	96
23.	100	82	8	20	57	61
24.	100	90	16	35	71	114
25.	100	87	16	33	71	120
Average:	100	86	12	26	63	96

TABLE 3

MCNP PERFORMANCE NORMALIZED TO IBM RS/6000-550

	IBM-550	YMP	XMP	Sun Sparc1	Sun Sparc2	HP-730
1.	100	191	160	20	41	158
2.	100	184	155	17	37	152
3.	100	140	122	20	45	156
4.	100	190	161	16	36	145
5.	100	191	161	14	34	143
6.	100	189	159	19	41	165
7.	100	163	141	21	44	167
8.	100	194	158	16	40	124
9.	100	138	120	21	44	162
10.	100	202	171	17	38	143
11.	100	136	125	16	37	152
12.	100	189	162	18	39	140
13.	100	125	109	17	39	165
14.	100	124	108	24	50	167
15.	100	160	140	24	48	185
16.	100	155	133	24	47	167
17.	100	159	134	18	39	143
18.	100	120	112	20	44	172
19.	100	201	174	25	53	167
20.	100	170	138	14	34	97
21.	100	167	147	21	42	149
22.	100	157	139	22	48	152
23.	100	177	146	14	36	107
24.	100	140	126	23	48	159
25.	100	141	123	23	47	169
Average:	100	164	141	19	42	152

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