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FEATURES AND PERFORMANCE OF MCNP4B

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ABSTRACT

MCNP4B was released for international distribution in February, 1997. We summarize the new MCNP4B features since the release of MCNP4A over three years earlier and compare performance. Then we describe new methods being developed for future code releases.

I. INTRODUCTION

The Monte Carlo N-Particle computer code, MCNP,™ version 4B, was released for international distribution by the Radiation Safety Information Computational Center (RSICC) in Oak Ridge, Tennessee, in March 1997. MCNP4B is the first release of MCNP since MCNP4A was released in November, 1993. MCNP4B has many important new features of value for simulating the interaction of radiation with matter. We present for the first time a comparison of MCNP4B and MCNP4A timing. We then describe a number of new Monte Carlo and MCNP research areas to enhance ex-core neutron response calculations and other applications in the future.

II. MCNP

MCNP[1] is a general-purpose Monte Carlo N-Particle radiation transport code. It transports neutrons from 0–100 MeV, photons from 1 keV–100 GeV, and electrons from 1 keV–100 GeV. The physics is fully continuous energy or multigroup with an adjoint option. Data sources include ENDF/B-VI continuous-energy isotopic neutron data, photon libraries, electron libraries, and multigroup data for any particle for which there is data. The geometry is fully three dimensional including all second-degree surfaces and fourth order tori. Fixed, eigenvalue (criticality k_{eff} estimators), surface and user sources are available. Output and sources are fully time-dependent. Tallies include surface, track-length, heating, point flux and pulse height estimators and may provide all energy, time, angle, and other dependency information. There is a wide variety of variance reduction options to significantly enhance Monte Carlo sampling efficiency and speed up calculations. There is an elaborate, standard statistical analysis capability to detect false convergence.

MCNP applications include radiation shielding and protection, reactor analysis, criticality safety, medical applications from boron neutron therapy to positron emission tomography, aerospace, physics, defense, environmental, and other applications ranging from drug interdiction to bulk materials processing.

III. NEW METHODS FOR NEUTRON RESPONSE CALCULATIONS WITH MCNP4B

MCNP4B has many improvements over MCNP4A. The major new features are:

1) Differential Operator Perturbations: The differential operator perturbation technique has been incorporated into MCNP4B for response perturbations related to cross-section data such as density and composition.[2] The differential operator perturbation capability should be an important step forward for neutron response calculations. Previously, if one wanted to calculate the effect of a small perturbation in a problem with MCNP, such as an ex-core detector for a nuclear reactor, the only way was to run two problems almost to convergence and then hope that the difference between the two problems was less than the statistical noise in the Monte Carlo simulation. With the differential operator perturbation capability, the difference caused by the perturbation is tallied directly with its own statistical error. MCNP uses the first and second order terms given by the Taylor series expansion. Higher-order terms are usually not required for perturbations less than about 30%, in which case the difference in two converged calculations is no longer difficult to separate from statistical fluctuations.

2) Enhanced Electron Physics: Landau energy loss straggling has been implemented for secondary electron energy and angle distributions along with photoelectric electron production improvements to upgrade the MCNP electron physics to the level of the Integrated Tiger Series[3] (ITS) ver. 3. The improved electron scattering[4] is important for all electron problems.

3) PVM Load Balancing and Fault Tolerance: Multitasking with Parallel Virtual Machine (PVM)[5] software has been greatly enhanced by load balancing, which sends more particles to less busy or faster processors, and fault tolerance, which enables problems to continue even if some processors doing the problem become unavailable. Clusters of workstations can now be linked together to run a single calculation in parallel with PVM (Parallel Virtual Machine) public domain software. The ability to link clusters of PCs running PVM with LINUX (PC Unix language) is being investigated. If some PCs or workstations are slower than others, the load balance sends fewer particles to them so that calculations are not limited by the slowest node on the system. If one

machine crashes, then the fault tolerance enables other machines on the network to replace it so the entire calculation is not lost as in MCNP4A.

4) Cross-Section Plotting: All cross sections of nuclides or mixed materials used in a problem can be plotted as a standard MCNP4B feature. Secondary energy and angular distributions are not plotted, but all reactions cross sections, heating numbers, and stopping powers are. The new MCNP4B cross- section plotting capability should be of interest to anyone wanting a better understanding of the physics in a problem. In particular, the ability to plot mixtures of isotopes and overlay different evaluations of a given cross section is very useful.

5) Software Quality Assurance: A Software Quality Assurance Plan[6] has been written consistent with the requirements of IEEE-730.1[7] and ISO-9000[8] software quality assurance standards. Further, the MCNP test set[9] and verification and validation procedures[10] have been significantly strengthened for even greater code robustness and reliability.

6) Repeated Structures / Lattice Geometry Improvements: (a) Electrons no longer get lost in repeated structures / lattice geometries. (b) Lattices and repeated structures may now have surfaces coincident with surfaces of cells at higher universe levels. In MCNP4A and earlier versions, users had to have surfaces at different universe levels specified an arbitrarily small distance apart so that they would not be coincident. This nuisance requirement is eliminated in MCNP4B. (c) Sources, collisions and tracks in each element of lattices and repeated structures geometries are now output instead of being reported at just the cell level. Consequently, adequate sampling can be verified and variance reduction parameters can be properly adjusted. This new summary of repeated structures / lattice activity also serves as a universe map for complicated geometries. These improvements in the repeated structures / lattice geometries are particularly useful for nuclear reactor applications where there are large arrays of lattices of fuel elements in the geometry.

7) Postscript Files: MCNP4B now writes postscript files of any plot generated by the code so that hardcopy plots can be easily made for postscript printers. The ability to generate postscript files of all geometry, tally, and cross-section plots on all systems is convenient, and very important on those systems, such as PCs, where MCNP plot images could not be stored or printed previously.

8) Lifetimes: Prompt neutron lifetimes[11] for any reaction are now available for both fixed source and criticality source calculations. Prompt neutron lifetimes are a fundamental parameter for the reactor kinetics equation and can also be important in oil-well logging problems to determine die-away times. The prompt neutron lifetime[12] is the neutron population (1/v times the neutron flux, where v is the neutron speed) divided by a reaction rate. The new MCNP4B 1/v tally multiplier,

problems with “*” still track MCNP4A exactly. The problems without the “*” will still converge to the same MCNP4A result but do not track identically because of bug corrections and new features, such as enhanced electron physics, which significantly affect the random walk. Even with new and improved physics, comparison of columns 3 and 4 indicates that running times per history are about the same.

TABLE I

COMPARISON OF MCNP4A AND MCNP4B RUNNING TIMES

Test Problem	MCNP4A time	MCNP4B tracking	MCNP4B non-track
1	0.07	0.07	0.07*
2	0.25	0.25	0.25*
3	0.59	0.60	0.59
4	0.55	0.55	0.51
5	0.32	0.33	0.30
6	0.16	0.16	0.16*
7	0.56	0.57	0.57*
8	0.27	0.29	0.28
9	0.29	0.29	0.29*
10	0.14	0.15	0.14
11	0.33	0.34	0.35
12	0.87	0.89	0.92
13	0.38	0.38	0.38*
14	0.45	0.44	0.44*
15	0.09	0.09	0.09*
16	0.62	0.58	0.58
17	0.25	0.26	0.27
18	0.92	0.67	0.67
19	0.36	0.37	0.37*
20	0.49	0.54	0.56
21	0.31	0.32	0.32
22	0.34	0.35	0.35
23	0.38	0.42	0.42
24	0.67	0.53	0.54
25	0.19	0.19	0.19*

along with the existing capability to calculate any reaction rate, now provides a means of computing any prompt neutron lifetime in any problem as an option with a track length estimator. Collision estimators of the removal, capture (n,0n), fission, and escape lifetimes are automatically computed for criticality source problems.

9) HMCNP: All the capabilities of the HMCNP module of the LAHET Code System[13] have been incorporated into MCNP4B to eliminate the need for a separate HMCNP code. The integration of the LAHET Code System (LCS) HMCNP code into MCNP4B is very significant for high-energy problems transporting protons, neutrons, and other particles above 20 MeV.

In addition, MCNP has been ported to a number of new systems and architectures. PC X-windows on the PC was enabled using MetaWare High C 3.3, DESQview/X 2.0 with the MetaWare X11 toolkit. MCNP4B also works with Windows 95 and Windows NT. Corrections for the Cray T3D have been made. Modifications have been incorporated for 64-bit scientific workstations, particularly the DEC Alpha and the SGI Power Challenger. Multiprocessing can be performed across processors in a multiprocessor workstation.[14]

IV. TIMING COMPARISON OF MCNP4A AND MCNP4B

What is the effect on problem performance of adding many significant new features to MCNP4B? We present here for the first time a comparison of MCNP4B running times to MCNP4A. All calculations were done with the MCNP4A test set, because MCNP4A cannot pass the MCNP4B test set since the MCNP4B test set reflects all bugs corrected in MCNP4A and also tests new features in MCNP4B. All calculations were performed on a single computing platform (Cray YMP). Both MCNP4A and MCNP4B were compiled with the same compiler in the same environment. All problems were run multiple times in identical environments: the numbers presented are averages of those times. MCNP4B has a “tracking switch” so that it tracks MCNP4A exactly for quality control purposes. This tracking switch even adds back in MCNP4A bugs so that MCNP4A problems give identical results to those run with MCNP4B. Therefore, it was possible to make an exact, fair comparison of the running times of MCNP4A to MCNP4B.

The results are presented in Table I. Column 1 is the test problem number. Column 2 gives the Cray YMP running time in minutes for the 25 MCNP4A test problems. Column 3 gives the Cray YMP running time in minutes for the same problems run with MCNP4B but with the tracking switch turned on so that each problem ran exactly the same random walks and had the exact same results. MCNP4B is seen to be slightly slower than MCNP4A for most problems and significantly faster for a few where new features have cleaned up old parts of the code (test problems 18 and 24, both criticality problems with repeated structures / lattices). Column 4 shows the MCNP4B results if the tracking is not turned on. The

V. FUTURE MONTE CARLO METHODS FOR NEUTRON RESPONSE CALCULATIONS WITH MCNP

MCNP has an active research and development program. Work is already underway on new features for the next code version.

The unresolved resonance range probability table method is a better way of representing neutron physics above the resolved resonance range. The unresolved resonance range is where the neutron cross-section resonances are so close together that the neutron cross section is represented by an average cross section because the individual resonances cannot be resolved. The probability table method represents these unresolved resonances with probabilities rather than their average value, so the average cross section at any energy within the range is still the same, but the sampled cross section may be significantly higher or lower. This better representation of the physics can make a difference for hard-spectrum problems where resonance self-shielding in these higher energy ranges is important. Resolved resonances can also be represented by probability tables, thereby decreasing storage requirements for nuclides with many resolved resonances close together. For thermal reactors the improvement should not be noticeable. Completion of the unresolved resonance range capability is scheduled for late 1997.

Another major project is merging LAHET with MCNP. MCNP would track over thirty different particle types at very high energies in a self-consistent way which is important for accelerators and other high-energy applications. A prototype version of the merged code is expected by March 1997.

Work is also underway on the AVATAR™ automatic variance reduction and graphical user interface project.[15] Choosing good variance reduction parameters for large and complicated geometries such as nuclear reactors is presently very difficult; an automated means would be very useful for neutron response calculations and nearly all other radiation transport problems. Further, MCNP presently limits geometric variance reduction to problem cells, and the AVATAR capability would also allow setting variance reduction parameters for a superimposed importance grid overlaying the physical geometry. Thus, geometries would not have to be geometrically subdivided for variance reduction purposes; the superimposed grid would be used when it is better. Finally, a graphical user interface would greatly enhance the ease of setting up large problems, particularly ex-core neutron response calculations. A prototype AVATAR graphical user interface capability has been produced. Users can set up many (but not all) kinds of MCNP problems with the point-and-click graphics code JUSTINE.™ Then with the push of a button, the DANTSYS[16] three-dimensional THREEDANT code is run to produce adjoint fluxes which are input into MCNP as importances.

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Perhaps the most ambitious research program related to MCNP is "Monte Carlo for the 21st Century" which is described on the MCNP World Wide Web site http://www-xdiv.lanl.gov/XTM/proj. The goal is to achieve exponential convergence, as opposed to the $\frac{1}{\sqrt{N}}$ (where N is the number of Monte Carlo histories, or statistical trials) convergence which now limits all Monte Carlo calculations. Promising results have already been demonstrated in prototype limited-purpose codes for simple problems. The $\frac{1}{\sqrt{N}}$ limitation is overcome by adaptive learning. As the problem progresses it "learns" how to better set variance reduction importance functions and changes its sampling algorithms. Exponential convergence would allow high-accuracy Monte Carlo calculations with quick convergence, greatly increasing the usefulness of the Monte Carlo method for all applications.

VI. CONCLUDING REMARKS

In summary, the first new MCNP version in over three years, MCNP4B, has just been released. It contains a number of important features for Monte Carlo radiation transport applications. Despite the new features and increased size of the code, running times do not appear to be significantly increased, as shown here for the first time. Work is already underway on new capabilities for future MCNP versions including better unresolved resonance range neutron physics, high-energy many-particle physics, automatic variance reduction and easier user problem setup with AVATAR and the JUSTINE graphical user interface, and a revolutionary advance in the Monte Carlo method itself: exponential convergence.

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