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Title:

Performance Enhancements of MCNP4B, MCNP5, and MCNPX for Monte Carlo Radiotherapy Planning Calculations in Lattice Geometries

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Performance enhancements of MCNP4B, MCNP5, and MCNPX for Monte Carlo Radiotherapy Planning Calculations in Lattice Geometries

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Abstract

Achieving reasonable computation times for Monte Carlo-based radiotherapy planning calculations while simulating enough histories to maintain acceptable statistical precision can be difficult, especially for the computationally expensive, scatter-dominated neutron transport problems required for Neutron Capture Therapy (NCT). Several NCT treatment planning systems (TPS) employ the general-purpose Monte Carlo radiation transport code MCNP as their dose computation engine because of its many advantages. This paper examines the issue of computational speed for 3 versions of the MCNP code, MCNP4B, MCNP5, and MCNPX, in the context of NCT treatment planning calculations using a voxel phantom produced by the NCTPlan TPS. In addition to the standard versions of these codes, patched versions of MCNP4B and MCNP5 specially accelerated for calculations in a lattice geometry were assessed. Furthermore, the influence of different geometric representations (cell or lattice representations of the voxel model) and tallying techniques, including the recently developed mesh tally, on computation efficiency was assessed. For certain combinations of geometric representation and tally techniques, the computations are prohibitively slow, taking more than 8,000 minutes per million source neutrons and photons. For the problem studied, the minimum total computation times of 12.3 and 16.2 min were obtained using the patched versions of MCNP4B and MCNP5, respectively, with a lattice geometry for 10^6 neutron and 10^6 photon histories. Using the standard, unpatched versions of MCNP, computation times only 23-71% slower can be obtained by using a judicious combination of geometric representation and tally technique to avoid prohibitively slow computations. Compared to the slowest calculations, calculations using the patched version of MCNP4B and MCNP5 represent 530- to 660-fold improvements in speed. These studies may provide useful guidance for others who are using MCNP for radiotherapy planning calculations or other applications with similar voxel or lattice geometries.

Key words: Boron Neutron Capture Therapy (BNCT), Monte Carlo radiation transport, radiation therapy planning calculations, MCNP (Monte Carlo n-Particle)

1. Introduction

The general-purpose radiation transport code MCNP (X-5 Monte Carlo Team, 2003) from Los Alamos National Laboratory (LANL) has been used since the early 1990s (Zamenhof, 1990, 1996) as the dose computation engine in treatment planning systems for Neutron Capture Therapy (NCT). These planning systems, generally employing customized voxel models of the patient derived from medical image data, include NCTPlan (González, 2002, Kiger, 2002) and MacNCTPlan,(Kiger, 1996) developed at Harvard-MIT and CNEA, JCDS, developed at JAERI,(Kumada, 2001, 2002) and BDTPS developed at the University of Pisa and JRC Petten,(Cerullo, 2004) and the MiMMC planning system under development at Harvard-MIT.

The MCNP code is an obvious choice for simulating radiation transport for NCT treatment planning. MCNP is highly developed, with detailed physics models for neutron, photon and electron interactions, representing more than 500 person-years of development, and is very well benchmarked and widely used. Also, for a radiation transport code, it is very user-friendly. MCNP is also very frequently used for reactor modeling, neutron beam design, and computation of the radiation source description for NCT treatment planning calculations. MCNP's very flexible source definition facility and its capability to record and later read and transport individual particles is also an advantage for treatment planning calculations where it is desirable to avoid making significant approximations in the source term. For specific problems, however, MCNP's generality could be a disadvantage and, as is frequently the case with Monte Carlo simulations, speed is an important issue.

A patch for MCNP4B was developed to accelerate for BNCT treatment planning problems by LANL in collaboration with the Harvard-MIT NCT group in 1997.(Goorley, 1998a, 1998b, 2001) By employing tracking and tallying algorithms specific to the voxel geometry, this modification, known as the 'speed tally patch,' makes the computations significantly more efficient. This patched version of MCNP4B has been used in planning NCT treatments of over 25 patients at Harvad-MIT.(Palmer, 2002, Kiger, 2004) A similar patch affecting only the tally subroutine has been recently developed for MCNP5 and it will soon be integrated into the next patched release of MCNP5, MCNP5_RSICC_1.30.(Goorley, 2004) Some improvements in lattice tally capabilities have already been made to MCNPX, incorporated into version 2.5d.

Recent developments such as the mesh tally, introduced in MCNPX and MCNP5 to allow tallying in a mesh independent of the problem geometry, as well as the incorporation of lattice improvements in MCNPX and general advancement of the codes warrants examination of their computational efficiency. This paper evaluates the performance of different accelerated and standard versions of MCNP with different geometric representations and tallying techniques.

2. Methods and Materials

Both standard and modified (patched) versions of MCNP were employed in this study. Three standard versions of MCNP were MCNP4B,(Briesmeister, 1997) MCNP5,(X-5 Monte Carlo Team, 2003) and MCNPX v. 2.5e (Waters, 2002, Hendricks, 2004). Patched versions of MCNP4B and MCNP5 specifically accelerated for computations in lattice geometries were also used. Each code was compiled with the Compaq Visual Fortran Compiler v. 6.6B using level 5 optimization except for MCNPX, which was compiled with level 4 optimization, the default setting for its build process. The unpatched versions of all codes passed their respective suites of test problems. The patched versions of MCNP5 and MCNP4B, however, crash when running their test suites as a result of the elimination of most of the tally subroutine.

When the lattice tally patch is integrated into the next MCNP5 distribution, this undesirable behavior will be fixed. Since only modifications to the tally routine were made, the patched version of MCNP5 produces identical particle tracks and uses the same random number sequence as the standard version of MCNP5 (i.e., particle transport is identical and unaffected by the patch).

The test problem used in this study was a calculation produced by NCTPlan of a cranial irradiation with the (now decommissioned) MIT M67 epithermal neutron beam; the geometry was a 21 x 21 x 25 cm array of 1 cm^3 voxels. Calculations for the single field entail one coupled neutron-photon simulation and one photon-only simulation. One million particle histories were simulated in each calculation except for those that were estimated to require more than 1000 min per 10^6 histories. For those cases, only 1000 histories were simulated for expediency and the results were linearly extrapolated to 10^6 histories.

Two different geometric descriptions of the voxel geometry were used in the calculations: cell geometry, where each voxel is an individual cell in the geometry or the lattice geometry, where each voxel is an element in a lattice. Two different tallying techniques were used in the runs as well: (F4) track length density tallies in the cells or lattice elements and mesh tallies. Mesh tallies are a new feature in MCNP5 and MCNPX that allow track length density tallies of flux or dose to be made in a mesh independent of the problem geometry. Thermal and fast neutron dose, boron dose, and photon dose were tallied using energy dependent kerma factors for ICRU brain composition reported by Goorley (2002). For a few runs, no tallies were used in order to evaluate the impact of tallies on computational efficiency.

All computations were performed on a single processor 1.8 GHz Pentium IV PC running Windows 2000. The start and stop wall-clock times of each simulation were recorded by scripts and the difference was reported as the calculation time. This was done because the CPU time used by the codes and reported in the output files can be significantly biased compared to the wall clock time by periods of partial usage of the CPU, e.g., reads and writes to virtual memory. Each simulation was run 5 times and the results were averaged to ensure that no unusual behavior (e.g., virus scans) affected or interrupted the simulations. The results varied little for each particular simulation; the mean and maximum coefficients of variation were 1% and 3.5%.

3. Results

Calculation times for 10^6 neutron and 10^6 photon histories are reported in Tables 1 and 2, respectively, for the 3 versions of the code using different combinations of geometric representations and tally techniques for this problem. Fig. 1 shows total calculation times for simulation of 10^6 neutron and 10^6 photon histories for the different combinations of codes, geometry, and tallies. The ordinate in Fig. 1 was truncated at 25 min to emphasize the variation between the faster code-geometry-tally combinations. Calculation times for three sets of simulations exceed 25 min. Notably, the total calculation times using MCNP4B and MCNP5 with the lattice geometry and the standard F4 tally are prohibitively slow, both in excess of 8100 min (> 5 days). A bug in the current version of MCNPX causes the code to crash when more than 2 mesh tallies for dose are used. For the neutron mode problems, 3 mesh tallies are required, so MCNPX could not be properly evaluated using this problem. Initialization times for the runs ranged from 0.24 to 0.6 min and depended on the code, tally and geometry type as well as the particles simulated in the problem.

4. Discussion

The fastest simulations times for each code were obtained using the lattice geometry and either the speed tally (MCNP4B and MCNP5) or the standard F4 tally (MCNPX). Interestingly calculations with standard F4 tallies in the lattice geometry with MCNP4B and MCNP5 are extremely slow, 530-660 times slower than the with the speed tally patch. MCNPX, on the other hand, already has some improvements to the lattice tally built into its code base, avoiding the excessively slow calculations of MCNP4B and MCNP5. Simulations using the standard, unpatched versions of MCNP4B and MCNP5 with the lattice geometry and no tallies were somewhat faster than the patched versions with the lattice geometry and tallies because of the small, but significant computational expense of the (speed) tallies. The fact that the standard MCNP4B and MCNP5 executables ran the lattice geometry quickly without tallies indicates that the inefficiency with the lattice geometry arises from tallies rather than particle tracking. Moreover, using the F4 tally, the standard MCNP4B and MCNP5 executables produce reasonable computation times with the cell geometry but are excessively slow for the lattice geometry. The fact that the same tally subroutine is used in each of these codes to tally in both the cell and lattice geometries and that fast computations are achieved without any tallies suggests that a particular aspect of the tally subroutine relevant only to lattice geometries is responsible for the inefficiency.

Because of a bug in the MCNPX, the computational efficiency and potential advantage of the mesh tally could not be fully explored. With MCNP5, however, the mesh tally with the lattice geometry offers only a slight speed advantage over the cell geometry and F4 tally in the problems studied, but a great advantage over the very slow lattice geometry with the F4 tally. The cards used for the mesh tallies with MCNP5 are provided in the Appendix. The lattice geometry offers an efficient representation of the voxel model, especially when the number of voxels is very large, e.g., more than 10^4. Since the speed tally patch replaces most of the tally subroutine with a very efficient segment of compact code, some tally options, e.g., energy binning and integration of the flux spectrum against cross sections, are lost when using the speed tally patch. The mesh tally in MCNP5 represents a reasonably efficient alternative to the speed tally patch that retains this functionality. Moreover, when the tally mesh is identically coincident with the geometric lattice, results for the mesh and lattice (F4) tallies are identical.

For a given combination of geometry and tally technique, MCNP4B was generally the fastest code and MCNPX the slowest. The patched version of MCNP4B is expected to be slightly faster than the patched version of MCNP5, since the MCNP4B version contains modifications to both the tally and tracking routines, while the patched version of MCNP5 contains only modifications to the tally routine. MCNP5 may also be slower than MCNP4B in part because of its conversion from Fortran 77 to Fortran 90. It is likely that extra computational overhead needed for all-particle transport, one of the many extended capabilities of MCNPX, makes it somewhat slower than the other two codes. Also, the difference in compiler optimization levels used between MCNPX (level 4) and MCNP4B and 5 (level 5) may have an impact on speed, but we expect that this difference to be small.

The problems examined in this study were fixed source calculations of neutron and photon transport through a voxel model of a human head with calculation of multiple dose components. The results of this analysis may be relevant to other applications of MCNP that employ a lattice geometry, e.g., reactor simulations. It is hoped that this analysis will provide useful guidance for others using MCNP for similar applications.

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Table 1. Calculation times in minutes per million neutron histories for different combinations of geometric representation and tally technique using the 3 versions of MCNP. Calculations using the speed tally used separate, patched executables rather than the standard versions of MCNP4B and MCNP5.

Geometry	Tally	MCNP4B	MCNP5	MCNPX
Cell	F4	12.0	15.0	36.3
Cell	Mesh		16.1	*
Cell	None	8.7	10.9	21.8
Lattice	F4	6913	7483	16.9
Lattice	Mesh		15.4	*
Lattice	Speed Tally	9.7	13.0	
Lattice	None	6.7	9.9	10.6

*The current version of MCNPX has a bug that causes it to crash when using more than 2 mesh tallies for dose. Three dose tallies are required for these neutron problems, preventing the use of MCNPX.

Table 2. Calculation times in minutes per million photon histories for different combinations of geometric representation and tally technique using the 3 versions of MCNP. Calculations using the speed tally used separate, patched executables rather than the standard versions of MCNP4B and MCNP5.

Geometry	Tally	MCNP4B	MCNP5	MCNPX
Cell	F4	5.2	5.0	17.4
Cell	Mesh		5.3	16.6
Cell	None	4.5	4.3	15.5
Lattice	F4	1230	1140	4.2
Lattice	Mesh		3.7	3.7
Lattice	Speed Tally	2.7	3.2	
Lattice	None	2.2	2.5	3.1

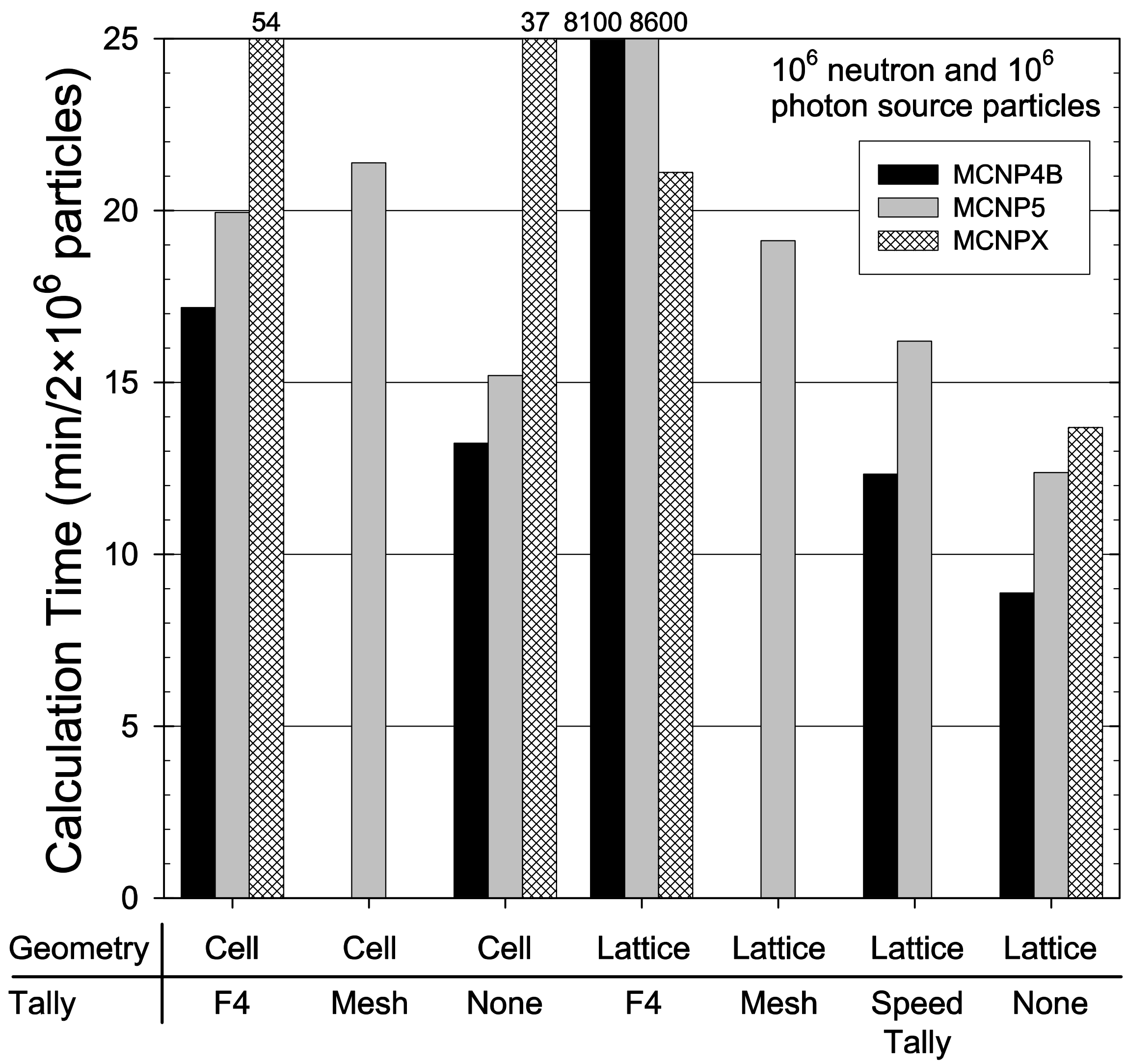

Fig. 1. Comparison of total (neutron + photon) calculation times for the 3 codes for different combinations of geometric representation and tally technique. Calculations using the speed tally were done with a separate, patched executable.

Appendix

Mesh tally cards used in MCNP5. Most values of the dose energy/dose function cards are omitted for brevity.

```
fm14        1.81468E+12
fm24        1.81468E+12
fm34        1.81468E+12
fmesh14:n   geom xyz  origin=-10.5 -10.5 -12.5
            imesh=10.5  iints=21
            jmesh=10.5  jints=21
            kmesh=12.5  kints=25
fmesh24:n   geom xyz  origin=-10.5 -10.5 -12.5
            imesh=10.5  iints=21
            jmesh=10.5  jints=21
            kmesh=12.5  kints=25
            emesh  0.5e-6 20.0
fmesh34:p   geom xyz  origin=-10.5 -10.5 -12.5
            imesh=10.5  iints=21
            jmesh=10.5  jints=21
            kmesh=12.5  kints=25
c
c
#            de14           df14
         1.000E-11       4.36034E-12
…
      (omitted for brevity)
…
         2.000E+01       6.48848E-18
c
c
#            de24           df24
    1.00000E-10     2.84836E-12
…
      (omitted for brevity)
…
    2.00000E+01     7.03169E-11
c
c
#            de34           df34
1.00000E-03              5.90571E-10
…
      (omitted for brevity)
…
2.00E+01                 4.37080E-11
c
```