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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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Harvard - MIT NCT Program

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 poster 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.

In addition, this poster examined the computational expense of decreasing the voxel size. Decreasing the voxel size does not dramatically affect the transport time; reducing the voxel size from 10 mm to 3 mm increases the transport time by factors of 2.0 for neutrons and 2.7 for photons. Problem initialization time, however, dramatically increases for smaller voxels, probably because of the large number of volumes tallied. For simulation of 10^6 histories, transport time and initialization time are approximately equal for the 4 mm voxel model. Significant improvements in the initialization time should be possible.

Fixed Geometry Timing Study Objectives

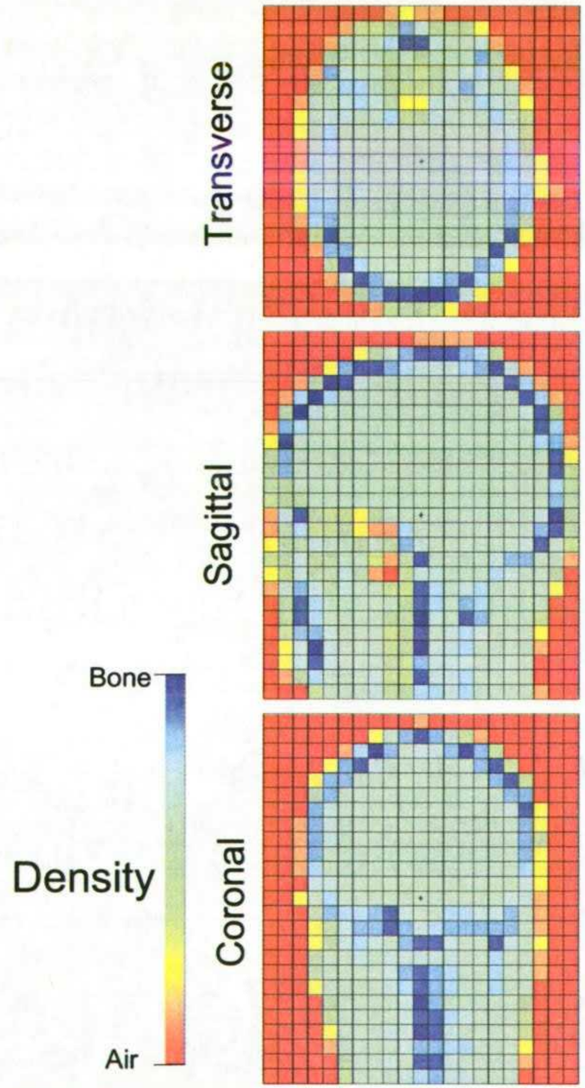
The objective is to quantify improvements in computational speed possible for NCT treatment planning problems for voxel models using different:

- Geometric representations
  - Cell representation (each voxel is represented by a cell)
  - Lattice (each voxel is an element in a lattice)
- Tally Techniques
  - Standard F4 tally using track length density estimate of flux
  - Speed Tally (i.e., F4 tally using the speed tally patch)
  - Mesh tally
- Transport Codes
  - MCNP4B
  - MCNP5
  - MCNPX

Fixed Geometry Timing Study Problem

- Voxel model constructed by NCTPlan
- 21 x 21 x 25 matrix of 1 cm^3 voxels
- MIT M67 neutron beam source used
- 10^6 neutrons and 10^6 photons simulated (in separate runs)
- Thermal neutron, fast neutron, boron, and incident and induced photon doses tallied
- Problems run on a 1.8 GHz Pentium 4 computer with 256 MB RAM

NCTPlan Model



Neutron Run Calculation Times

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

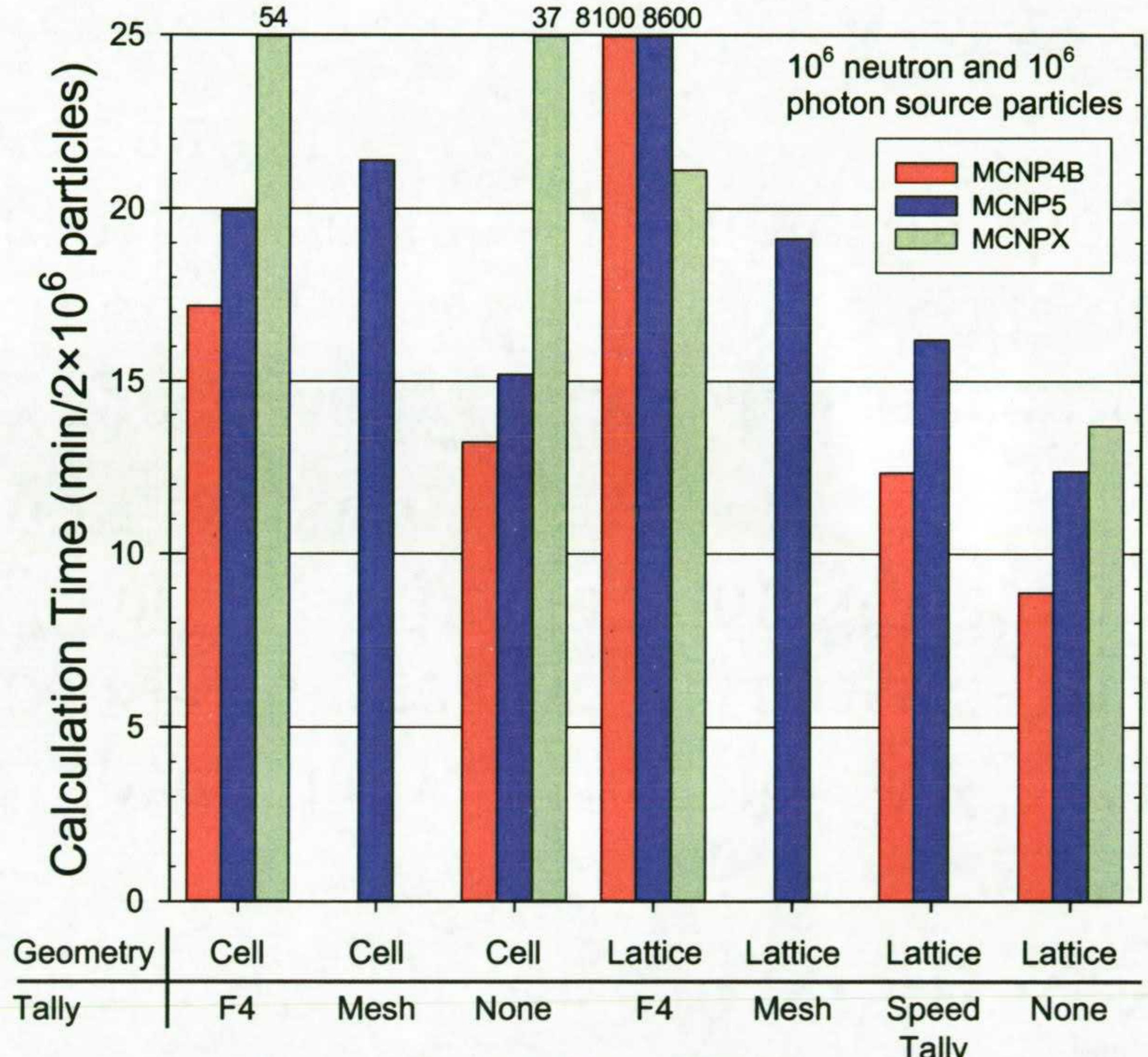
*The current version of MCNPX has a bug that causes it to crash when using more than 2 mesh tallies for dose. Three dose tallies are required for these neutron problems, preventing the use of MCNPX.

Photon Run Calculation Times

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

Effect of Geometry Definition and Tally Technique on Computation Time (Neutron + Photon Runs)



Speed Tally Patch for MCNP4B & MCNP5

- The speed tally patch for MCNP4B has been used clinically at Harvard-MIT since 1997 and is available with NCTPlan as well as from LANL
- The speed tally patch has recently been incorporated into the MCNP5 code base and is in a new patch available on the MCNP home page at

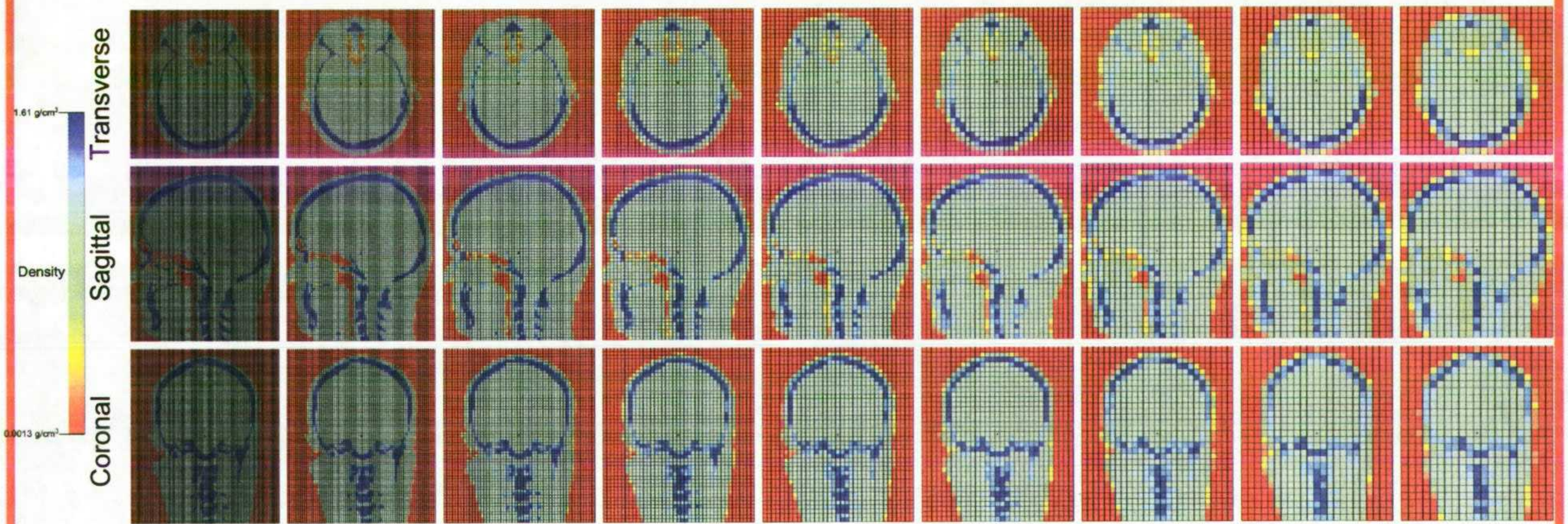
  http://laws.lanl.gov/x5/MCNP/resources.html

Voxel Size Timing Study

- Objective: to determine the computational cost of increasing the spatial resolution of the geometry and dose by reducing voxel size
- Models constructed by the MiMMC (Multi-Modal Monte Carlo) Planning System (see poster CP3)
- Outer dimensions of voxel models fixed at 210 x 210 x 250 mm
- Voxel size varied from 2 mm to 10 mm in roughly 1 mm increments
- 10^6 neutrons and 10^6 photons were run for each model using MCNP5 with the speed tally patch
- MIT M67 neutron beam source used
- Total time for calculation, initialization time (cp0), and transport time (total time minus initialization time, which is essentially the time spent transporting particles) were recorded
- Problems run on a 3.2 GHz Pentium 4 computer with 508 MB RAM

Variable Size Voxel Models

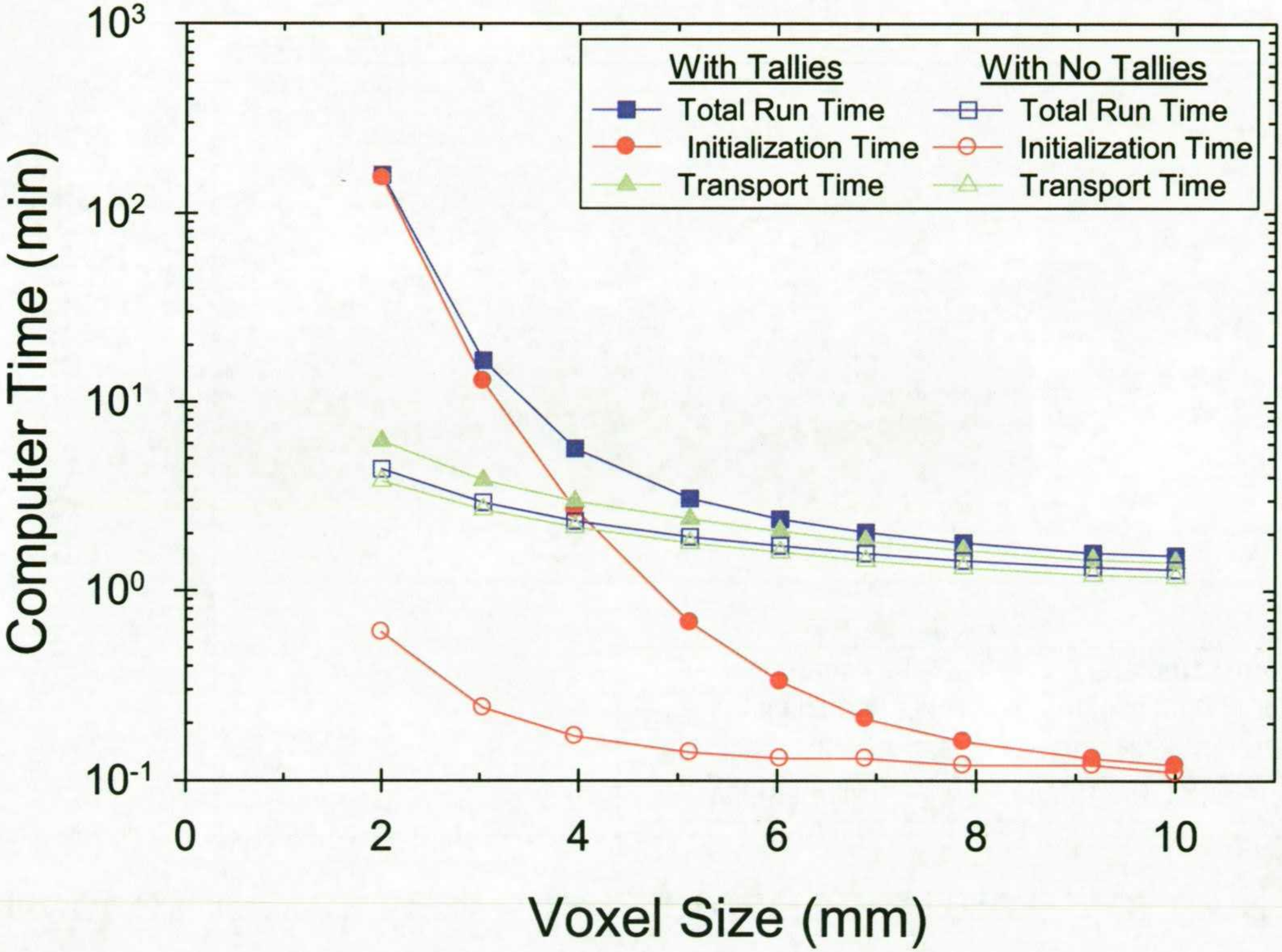
← Decreasing voxel size



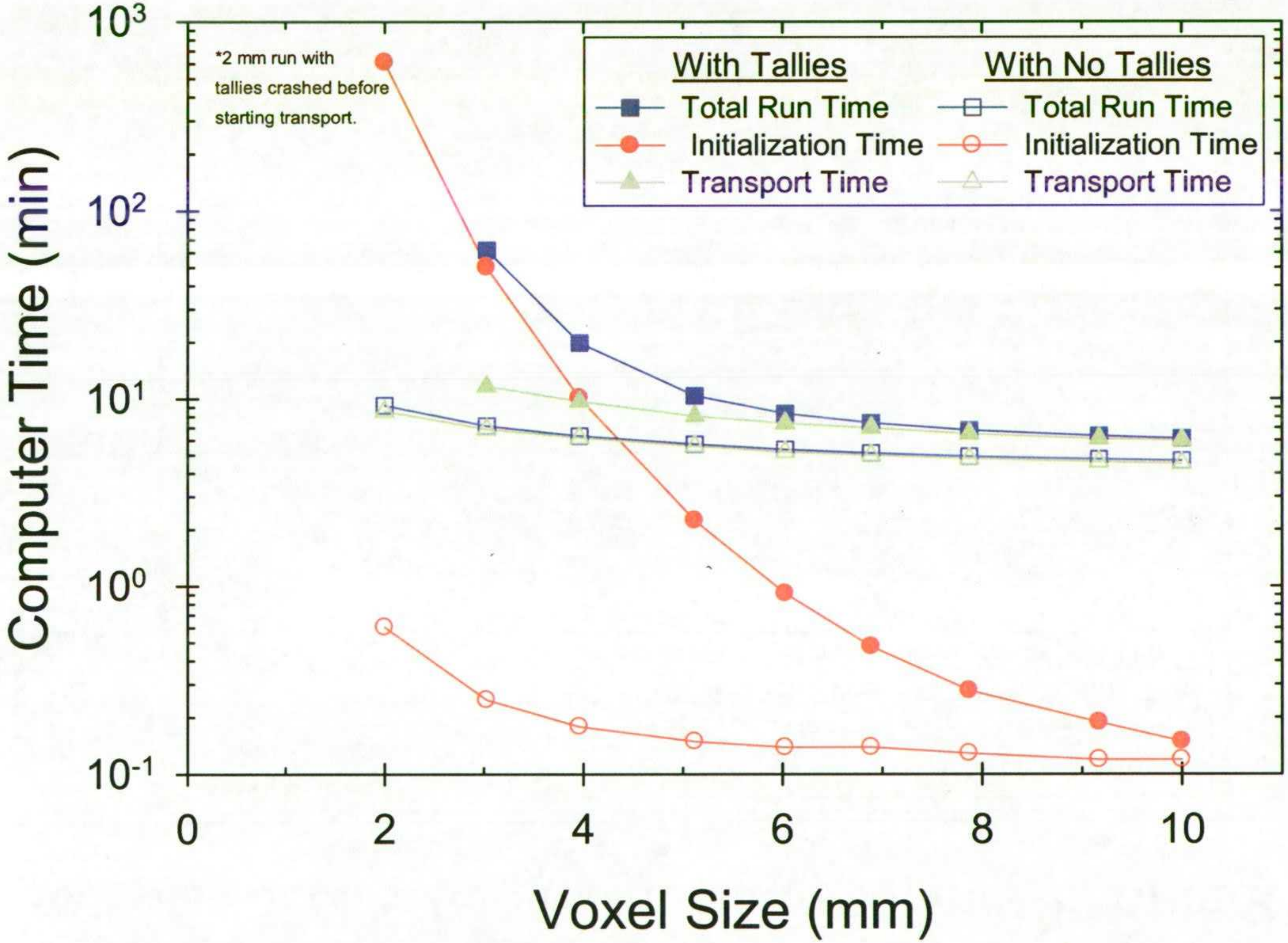
RMS Voxel Size (mm)	2.0	3.0	4.0	5.1	6.0	6.9	7.9	9.2	10.0
Number of Voxels	1378125	395163	176967	82369	50225	33635	22599	14283	11025
ΔX (mm)	2.0	3.043	3.962	5.122	6.000	6.774	7.778	9.130	10.0
ΔY (mm)	2.0	3.043	3.962	5.122	6.000	6.774	7.778	9.130	10.0
ΔZ (mm)	2.0	3.012	3.968	5.102	6.098	7.143	8.065	9.259	10.0

Total volume of voxel model constant: 210 mm x 210 mm x 250 mm

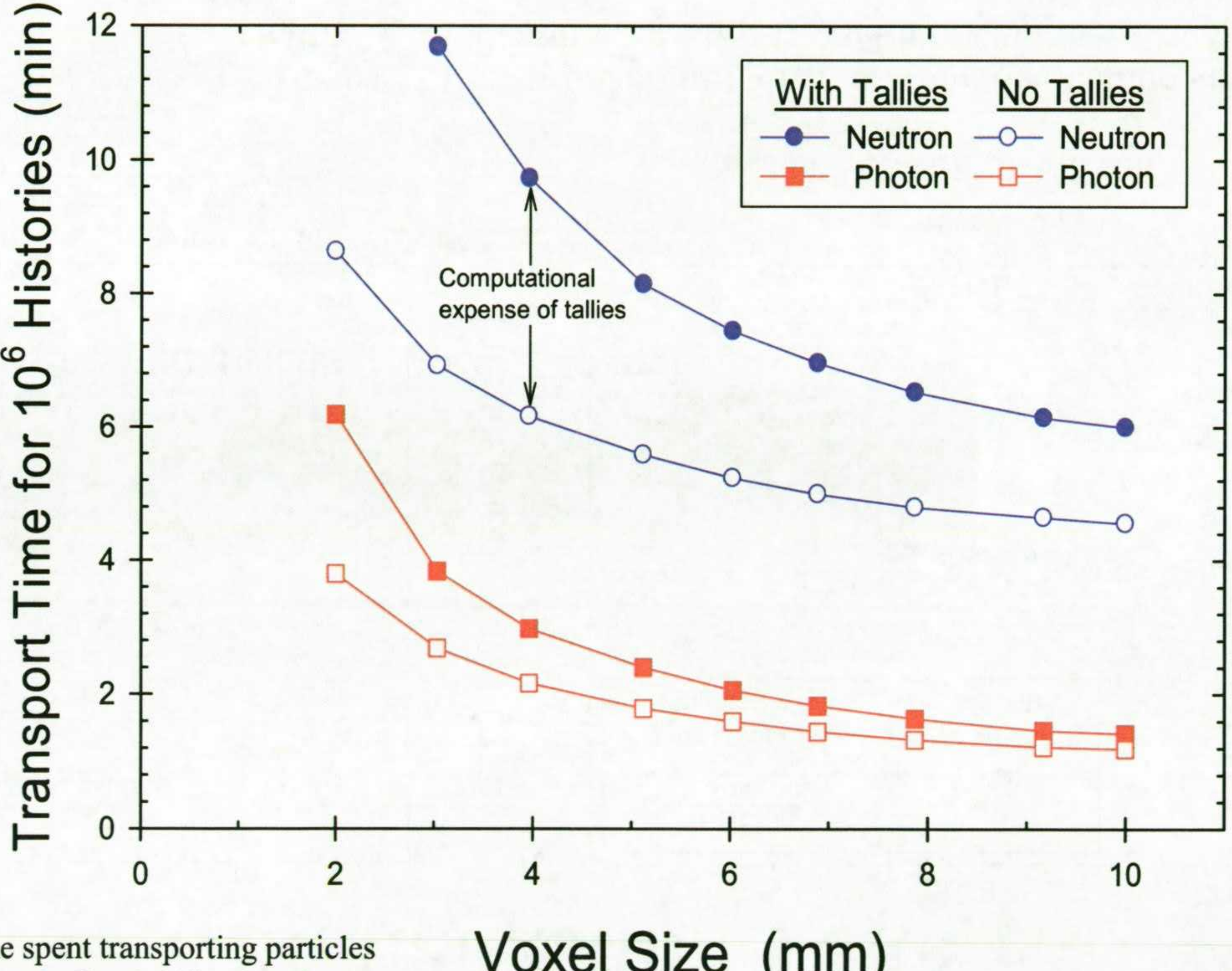
Effect of Voxel Size on Calculation Time--Photon Run



Effect of Voxel Size on Calculation Time--Neutron Run

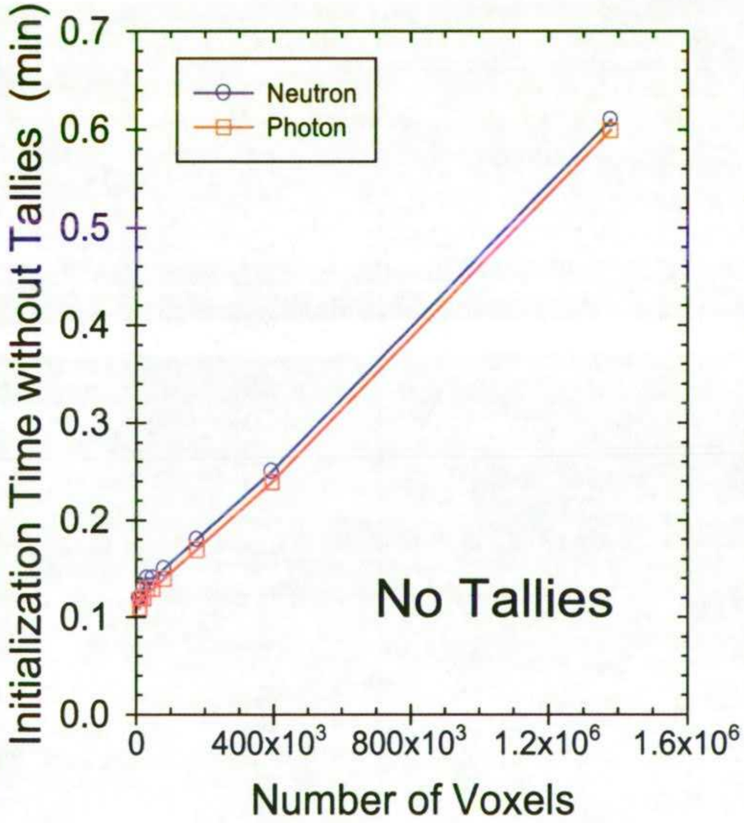


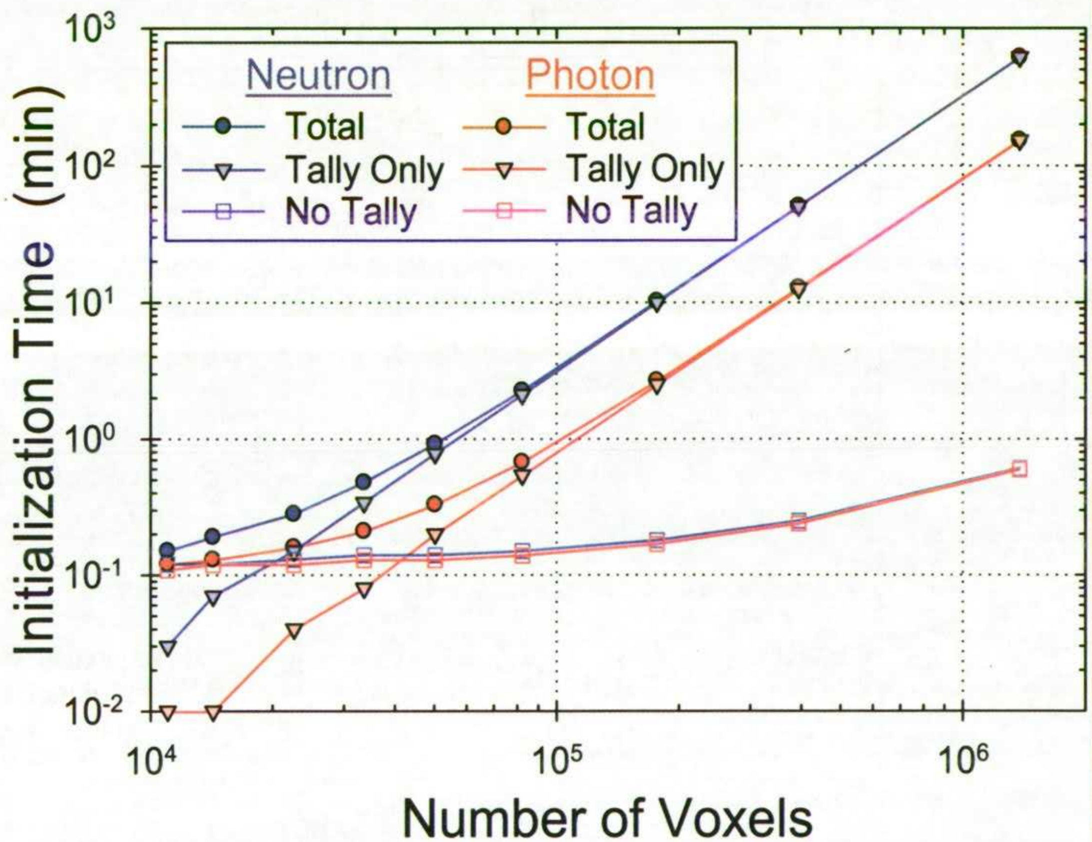
Effect of Voxel Size on Transport Time*



*Time spent transporting particles (i.e., excluding initilization time).

Initialization Time





$T_{NonTally} \propto O(N)$
- The part of the problem initialization time that is independent of tallies is small and varies linearly with the number of voxels

$T_{Tally} \propto O(N^2)$
- Initialization time due to tallies is proportional to the square of the number of voxels and can be extremely long

Conclusions

Detailed results are problem dependent, but several general conclusions may be drawn:

- Tallies and their initialization time have a profound impact on the speed of voxel model calculations
- Some combinations of geometric representation, tally technique, and code version are prohibitively slow (>8000 min/million source neutrons and photons)
- Judicious selection of geometric representation, tally technique, and code version provides good computational speed (12-16 min for 1 million neutron and 1 million photon histories on a somewhat dated 1.8 GHz PC)
- Decreasing the voxel size does not dramatically affect the transport time; reducing the voxel size from 10 mm to 3 mm increases the transport time by factors of 2.0 for neutrons and 2.7 for photons
- Problem initialization time, however, dramatically increases for smaller voxels, probably because of the large number of volumes tallied. Transport time and initialization time are approximately equal for the 4 mm voxel model for 10^6 histories. Significant improvements in the initialization time should be possible.

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