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Optimized Computation of Radiation Transport in Complex Multi-material Targets

L. Varga and E. Horvath

Defence R&D Canada
TECHNICAL MEMORANDUM
DREO TM 2001-069
November 2001

National Defence Défense nationale

Canada

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Optimized Computation of Radiation Transport in Complex Multi-material Targets

L. Varga
Defence Research Establishment Ottawa

E. Horvath
Jera Consulting

Defence Research Establishment Ottawa

Technical Memorandum

TM 2001-069

November 2001

Abstract

Traditionally, the complexity and statistical accuracy of radiation modelling has been limited by the execution time. For reliable results a large number of cases must be run to obtain good statistical results. In this work we have made some changes to the 3D Monte Carlo code "ACCEPT" to improve the execution speed for complex targets. Significant decrease in computational time has been achieved without changing the statistical accuracy of the results.

Résumé

Traditionnellement, la complexité et l'exactitude statistique de modeler de rayonnement a été limitée par le temps d'exécution. Pour des résultats fiables un grand nombre de cas doivent être exécutés pour obtenir de bons résultats statistiques. Dans ce travail nous avons fait quelques changements au code de 3D Monte Carlo " ACCEPT " pour améliorer la vitesse d'exécution pour les cibles complexes. L'augmentation significative de vitesse des calculs a été réalisée sans changer l'exactitude statistique des résultats.

Executive summary

Monte Carlo radiation transport codes, used for calculations of dose and charge deposition into specific targets, demand significant use of CPU time in order to obtain reasonable statistical accuracy of results. Without sacrificing the integrity of the results, the solution to reducing this execution time, besides increasing the CPU speed, is to make the code algorithm more efficient. We briefly describe the changes that were made to the 3D electron/photon Monte Carlo transport code "ACCEPT", to simulate dose and charge calculations into electronic components of a satellite and other targets. We compare the results with those of the original code.

In the Monte Carlo simulation process of the ACCEPT code, the code user can subdivide the target into equal sized geometrical bodies (subzones) by using the code's original input directive "ZSUB" if the target is composed of a single material. This directive is used when more accurate results are required, such as for example target depth/dose or depth/charge deposition profiles. The ZSUB directive works quite well for simple targets, however, in realistic situations where the target is an assembly of many objects of different materials; the code execution slows down considerably.

To remedy this problem, we have made changes to the code by adding a new directive, "ZMAT", to the "ACCEPT" module of the Tiger Series of Monte Carlo transport codes. The DREO developed ZMAT directive allows subdivision of a complex multi-material target into voxels (volume pixels) in the same manner as the ZSUB directive does for the single-material case. The saving in execution time comes from the routine, which determines the location of the radiation interaction during the transport inside the multi-material target.

Tests considering accuracy and speed of execution were performed between the original code and the modified version. The results obtained with the ZMAT modified code were identical to the original method, however, the timesavings with the ZMAT modified code increased significantly with the complexity of the target.

Varga L. and Horvath E. 2001.Optimized Computation of Radiation Transport in Complex Multi-material Targets. TM 2001-069. Defence Research Establishment Ottawa.

Sommaire

Les codes de transport de rayonnement de Monte Carlo, ont utilisé pour des calculs du dépôt de dose et de charge dans les cibles spécifiques, utilisation excessive de demande du TEMPS- CPU afin d'obtenir l'exactitude statistique raisonnable des résultats. Sans sacrifier l'intégrité de résultats, la solution pour réduire le temps d'exécution excessif, sans compter qu'augmenter la vitesse d'unité centrale de traitement, est de rendre l'algorithme de code plus efficace. Nous décrivons brièvement les changements qui ont été faits au code de transport de 3d electron/photon Monte Carlo "ACCEPT" que nous utilisons comme un outil pour simuler la dose et pour charger des calculs dans les composants électroniques d'un satellite et d'autres cibles. Nous comparons les résultats à ceux du code initial.

Dans le procédé de simulation de Monte Carlo du code de "ACCEPT", l'utilisateur de code peut subdiviser la cible en corps géométriques classés égaux (subzones) en utilisant l'entrée initiale " ZSUB " directif du code si la cible se compose de matériel simple. Cette directive est utilisée quand des résultats plus précis sont exigés, comme par exemple la cible depth/dose ou les profils de dépôt de depth/charge. La directive de ZSUB fonctionne tout à fait bien pour les cibles simples, cependant, dans des situations réalistes où la cible est un assemblage de beaucoup d'objets de différents matériaux, l'exécution de code ralentit considérablement.

Pour remédier à de ce problème, nous avons fait des changements au code en ajoutant une nouvelle directive, " ZMAT ", au " ACCEPT " le module de la série de tigre de codes de transport de Monte Carlo. La directive de ZMAT permet la subdivision d'une cible complexe de multi-matériel dans des voxels (Pixel de volume) de la même manière comme la directive de ZSUB fait pour le cas de simple-matériel. L'économie dans le temps d'exécution vient du sous-programme qui détermine l'emplacement de l'interaction de rayonnement pendant le transport à l'intérieur de la cible de multi-matériel.

Un test de précision et un nombre de vitesse des essais de comparaison d'exécution ont été exécutés entre le code initial et la version modifiée. Les résultats obtenus avec le code modifié par ZMAT étaient identiques à la méthode initiale, cependant, à l'épargne de temps avec le code modifié par ZMAT accru avec la complexité de la cible et devenu significatif.

Varga L. and Horvath E. 2001. Optimized Computation of Radiation Transport in Complex Multi-material Targets. TM 2001-069. Defence Research Establishment Ottawa.

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1. Introduction

For accurate results in radiation dose deposition calculations, scientists are often forced to turn to Monte Carlo techniques using complicated and realistic targets. This occurs since exact solution to the Boltzmann equation is, in general not known. Demand for statistically accurate results in dose deposition is understandable, for example, in the field of radiation therapy. However the accuracy of radiation dose estimates and the execution speed at which they are obtained are mutually opposing results. The result accuracy improves with higher resolution of target material definition or increasing the number of histories or both. Both solutions, however, place a disproportionate demand on CPU time. In order for these codes to become dose deposition prediction tools, such as for example in the area of radiation treatment design, the results of simulation must be available within a very short time, perhaps tens of minutes. Other applications can also benefit from a decrease in time for execution. Without sacrificing result integrity, the only way to reduce the excessive execution time, aside from increasing the CPU speed, is to make the code algorithm more efficient.

In this work, we briefly describe the new directive that we have added to the source code of the 3D-electron/photon Monte Carlo transport code "ACCEPT" in order to improve the execution time. This new directive is called "ZMAT" (Zoned Materials). The directive was tested against the original algorithm in several applications, during which the speed of execution and the final calculation results were compared.

2. The ZMAT Directive

A target in the Tiger Series of Monte Carlo radiation transport code is assembled by using the Constructive Solid Geometry technique. With this technique, the targets are assembled from basic (primitive) geometrical units (spheres, cylinders, cubes etc.) called "elements". During the code execution, after each element boundary crossing by the radiation particle, a routine identifies the element the particle had entered. By looping through the list of elements, the code identifies the element entered by matching the location of the particle with the co-ordinates of the element. In cases where high resolution is required, the target must be composed of a large number of small elements resulting in long execution time. Alternatively, the target can be composed of fewer, larger elements, but the elements themselves can be subdivided into subzones using the ZSUB directive. ZSUB directive provides the user with means of obtaining higher resolution results with minimum increase in execution time. This latter technique reduces execution time since there are fewer elements defined and a subzone in a given element is calculated in as few as three mathematical operations. The number of scenarios for which this technique is applicable limited since only homogeneous material regions can use the ZSUB directive.

Because of this limitation, we have developed a new directive, called "ZMAT", and incorporated it into the Tiger series "ACCEPT" code. The ZMAT directive functions in the same manner as the ZSUB directive except that it allows multi-material subdivision of a target. A separate specified file contains the material values in an array via table lookup. Each time a material value is required within the ZMAT divided body, it is obtained from the array. We have performed tests to show the viability of the ZMAT directive by comparing the results with these obtained with the unmodified code

3. Code Timing Tests

3.1 Cube Target

This test consisted of simulating irradiation of cubical targets with a monoenergetic unidirectional 1.25MeV Gamma ray beam. The targets were 3D arrays made up of smaller cube elements, the arrays size ranging from 10x10x10 to 60x60x60. The materials composing the elements were solids (steel, Aluminum, CsI and NaI), liquid (water), and gas (air). The simulation set-up is shown in Figure 1, showing the 10x10x10 case. The individual element size composing the target was kept constant at 4mm per side. The execution times required to complete 10^5 histories using the ZMAT modified and the original algorithm are listed in Table 1. It is evident that the ZMAT-modified algorithm execution time, relatively speaking, decreases with the increasing target complexity when compared with the original algorithm. The difference in results is attributed to the large number of loops that the original code must execute in order to

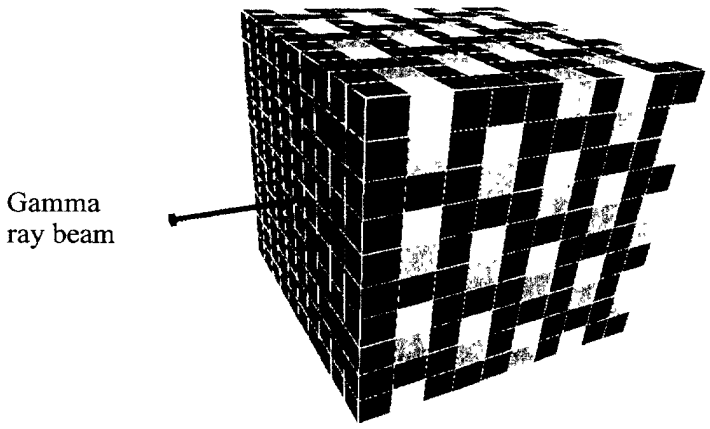

Figure 1. *Example of the block target composed of 10x10x10 elements, each 4mm per side. The Gamma ray beam is also shown.*

to identify the elements. The execution time using the ZMAT algorithm rises approximately linearly with the target dimensions whereas the execution time with the original algorithm rises at approximately the rate of the volume of the target. For low complexity scenarios, the execution times of the two methods are comparable.

Table 1. Execution Time Comparison

TARGET	NUMBER OF HISTORIES	EXECUTION TIME (s)		RATIO
Number of Elements		***ZMAT***	***ORIGINAL***	***zmat/original***
10x10x10	100 000	380	459	0.83
20x20x20	100 000	776	2349	0.33
30x30x30	100 000	1285	7904	0.16
40x40x40	100 000	1449	23467	0 06
50x50x50	100 000	1665	59363	0.028
60x60x60	100 000	2023	128173	0.016

3.2 VoxelMan Head

The 3D voxel (volume pixel) data of a human head was obtained from [1]. The head model, constructed from CT scans and MRI, is a 3D array containing 45x61x45voxels, including the void areas surrounding the head (each voxel is 0.4 cm on a side). The materials composing the target are water, water vapour and a complex combination of elements typically found in organic materials in the cranial area (skeleton cartilage, red marrow, trachea, adipose tissue (fat), cortical bone, blood, air).

For the tests, the radiation beam was, again, set to be mono-energetic (1.25 MeV) and mono-directional. The target/radiation beam set-up in the model is shown in Figure 2. The execution times as a function of number of histories is plotted in Figure 3. Orders of magnitude improvement in execution speed in complex scenarios involving large number of histories can be again observed with the ZMAT method.

We have also performed a comparison between the results generated by the original code and the ZMAT modified code. This is shown in Figure 4. This test shows that identical results are achieved with the two codes. In this figure, the total dose deposition as a function of depth obtained by the two methods is shown. The depth unit is a horizontal slice (numbered 1 to 45) through the target; each slice consists of 128 x 128 voxels.

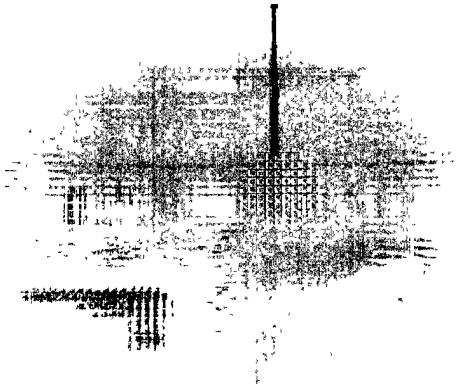

Figure 2. *VoxelMan head side view with the source position at the top*

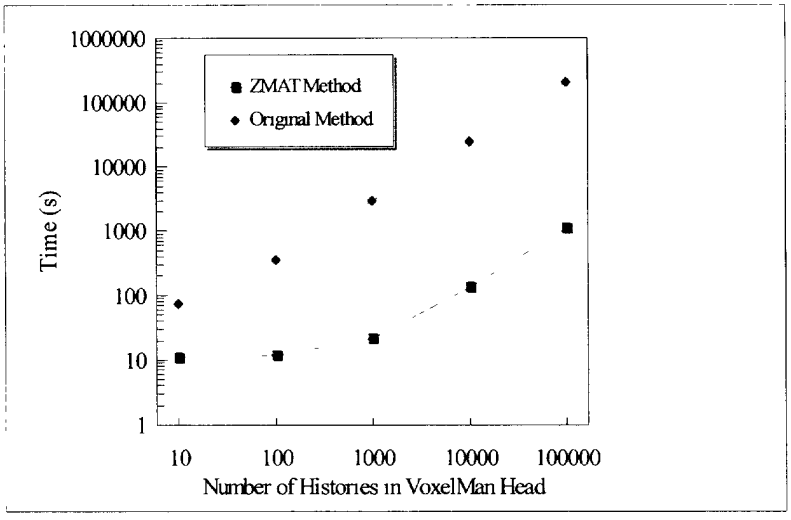

Figure 3. *Execution time comparison between the "Original" method and ZMAT method for the VoxelMan scenario*

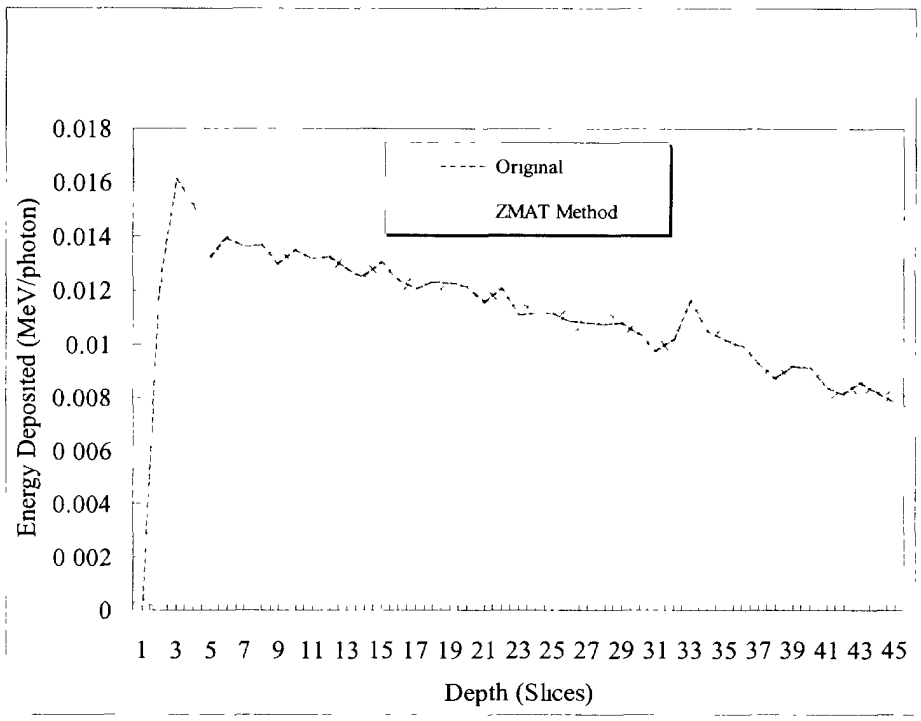

Figure 4. *Energy-depth deposition profile comparison between the two methods.*

4. Discussion

A new directive that increases the ITS Monte Carlo code execution speed has been introduced. The method is suitable for use in simulation scenarios where the target is composed of many elements of different materials. Once the number of elements reaches the thousands, the time saving can become substantial.

The calculation of a new element location is fast, requiring only 3 mathematical steps. The ZMAT processing operates similarly in concept to the ZSUB processing in the original code. The main difference is that each subzone may now have a unique material number associated with it. The method eliminates the costly searching through all defined elements that the original ACCEPT code must perform.

The new ZMAT coding tracks the current subzone with more accuracy than the original ITS. One test resulted in a "NO VALID DISTANCE" error in the original code, but with no such message using the ZMAT code. This may cause some minor differences in the results of the two techniques.

The use of ZMAT processing also simplifies the input specification. A single target can be defined that may contain tens of thousands of unique material specifications. The original method must define each material as a separate element with its own material specification. The overhead storage becomes excessive.

ZMAT processing is currently limited to Right Rectangular Parallelogram subzones. At this point, we do not consider this as a limitation, because a target composed of such elements is suitable to finite difference computations. As an example, the electron depositions into various subzones of the target provide information about the charge density that can be used in the Poisson equation solver to obtain the potential distribution inside the target. As a practical example, Figure 5 is the result of simulating the effect of electron radiation in space on an electronic board containing solid state electronic device among other things[2]. The target contains 100000 subzones of different materials (epoxy, copper etc.). The Figure shows the potential distribution caused by the electrons embedded inside the dielectric components of the board.

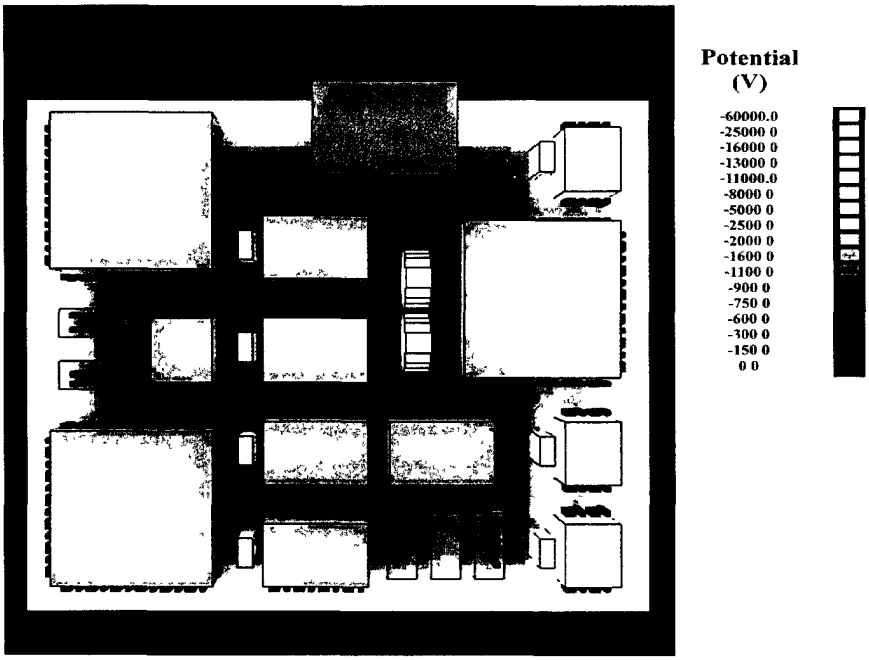

Figure 5. *Energy-depth deposition profile comparison between the two methods.*

5. Conclusion

Substantial increase of execution speed over the original code be can observed when using the code with the ZMAT directive. Simpler input files and fewer computational resources for storing of element structures has also been established with the ZMAT technique.

References

1. I.G. Zubal, Diagnostic Radiology, Yale University, Personal request.
2. L. Varga and E. Horvath, "Spacecraft 3-Dimensional Charge Deposition Modelling", RADECS 97 Conference Proceedings, Cannes, France, 1998.

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OPTIMIZED COMPUTATION OF RADIATION PROPAGATION IN COMPLEX MULTI-MATERIAL TARGETS (U)

4. AUTHORS (Last name, first name, middle initial)

Varga L. and Horvath E

5 DATE OF PUBLICATION (month and year of publication of document)	6a. NO OF PAGES (total containing information. Include Annexes, Appendices, etc.)	6b. NO. OF REFS (total cited in document)
November 2001	14	3

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Abstract

Traditionally, the complexity and statistical accuracy of radiation modelling has been limited by the execution time. For reliable results a large number of cases must be run to obtain good statistical results. In this work we have made some changes to the 3D Monte Carlo code "ACCEPT" to improve the execution speed for complex targets. Significant decrease in computational time has been achieved without changing the statistical accuracy of the results.

Résumé

Traditionnellement, la complexité et l'exactitude statistique de modeler de rayonnement a été limitée par le temps d'exécution. Pour des résultats fiables un grand nombre de cas doivent être exécutés pour obtenir de bons résultats statistiques. Dans ce travail nous avons fait quelques changements au code de 3D Monte Carlo " ACCEPT " pour améliorer la vitesse d'exécution pour les cibles complexes. L'augmentation significative de vitesse des calculs a été réalisée sans changer l'exactitude statistique des résultats.

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