2011 International Nuclear Atlantic Conference - INAC 2011
Belo Horizonte, MG, Brazil, October 24-28, 2011
ASSOCIAÇÃO BRASILEIRA DE ENERGIA NUCLEAR - ABEN
***ISBN:* 978-85-99141-04-5**

STUDY OF DISCRETE GEOMETRIC REPRESENTATION IN MCNP CODE

Paula C. G. Antunes[1], Paulo T. D. Siqueira[1], Gabriel P. Fonseca[1], Hélio Yoriyaz[1] and Vinícius A. Castro[1]

[1] Instituto de Pesquisas Energéticas e Nucleares (IPEN / CNEN - SP)
Av. Professor Lineu Prestes 2242
05508-000 São Paulo, SP
pacrisguian@gmail.com
ptsiquei@ipen.br
gabrielpaivafonseca@gmail.com
hyoriyaz@ipen.br
vcastro@ipen.br

ABSTRACT

The MCNP (Monte Carlo N-particle transport) is a computer code capable of simulating the interaction of radiation with matter and describing it in statistical methods with the most reliable representations of physical phenomena simulated. One of the highlights of this code over the other codes that also use the Monte Carlo method is its large geometric potential, that allows the manipulation of many volume elements (voxels) and the modeling of heterogeneous structures in three dimensions, because of its tool known as the *Repeated Structure*. The principle used in this technique is based on the ability to define a unitary structure called CELL once and repeat it several times, disposing it in a sequence so that to define a volume to be simulated, in three-dimensional, in the form of a matrix. In this context, the modeled structures are discretized, whose resolutions are determined by the user in the code input file. In order to understand and evaluate the quality of this tool and the possible interference in the estimates of absorbed dose calculations, this study proposes the modeling of an object of study using two different methodologies of description: the first using continuous surfaces pre-defined by the code and the second by the discretization of the object at different resolutions. The results enabled an accurate assessment of *Repeat Structure* feature, which is widely used to describe human anatomy in a realistic way in the radiation transport codes. This assessment will be applied, especially in the first millimeters of the volume elements, being this the region that represents the skin. This region adds complications to be represented on the code.

1. INTRODUCTION

The Monte Carlo method is a technique of the statistical numerical solution used to solve complex problems, especially, for those whose deterministic solution is extremely difficult or even impossible, due to the amount of variables involved in the problem, very common in real situations [1].

While deterministic methods solve problems with exact values, the Monte Carlo method solves with average values, based on techniques of sampling events whose probabilities of occurrence are known, from the drawing of random variables.

ISBN: **978-85-99141-04-5**

This methodology simulates the radiation interactions with matter, without an analytical description of the Boltzmann equation that governs the system. The physical phenomena are represented from the random sampling of the events described by Probability Density Functions (PDF) registered in the code [1].

The sampling of PDF provides knowledge of the possible events with a given particle. The particle trajectory, since its creation by the source until its their absorption by the medium, is known as the *history particle.*

The average behavior of a *history particle* determines a macroscopic physical quantity. As larger the number of *histories* processed, better is the average behavior of the system and consequently lower is the value of statistical uncertainty associated with the average value.

In this methodology have been based several radiation transport codes such as PENELOPE [2], EGS [3], ETRAN [4], MCNP [5], among others. Highlighting the MCNP code (Monte Carlo N-Particle) due to its large geometric flexibility that allows its use in areas that require the accurate data such as medical physics [6] and reactor physics [7].

The MCNP code was developed in the 50s by the researchers at Los Alamos National Laboratory, USA [5]. Its current version enables the transport of neutrons, photons, electrons, positrons, protons and heavy particles in systems with complex geometric details and flexibility in specifying the energy of transported particles [*8*].

The accuracy of the results obtained by the MCNP code is directly related to the degree of reality used in the geometry description to be studied. Similar geometry to the real provides results with more accurate.

This geometric description of the code can be accomplished in two ways: with continuous structures pre-defined by the code, which are inserted in the input files for mathematical expressions of simple geometrical figures such as planes, cylinders, spheres and ellipsoids; or discrete structures that allow the manipulation of many volume elements (voxels), with the aid of a tool known as *Repeated Structure*.

1.1 *Repeated Structure*

Repeated Structure is a tool of MCNP code that allows modeling of complex, irregular and heterogeneous structures in up to three dimensions [5]. As this feature makes it possible to describe only once the cells and surfaces of any structure that appears more than once in geometry.

The primary goal of the *Repeated Structures* capability is to enable reducing the amount of input data supplied by the user and the amount of computer memory needed by problems that have a lot of geometrical repetition. Problems that would be impractical because they take an unreasonable amount of work to set up or they use too much memory can be run, such as human anatomy.

2011 International Nuclear Atlantic Conference - INAC 2011
Belo Horizonte, MG, Brazil, October 24-28, 2011
ASSOCIAÇÃO BRASILEIRA DE ENERGIA NUCLEAR - ABEN
***ISBN:* 978-85-99141-04-5**

The principle used in this technique is capability to extend the concept of an MCNP CELL, which is modeling by the intersection of planes x, y and z, an unitary structure and repeat it several times, arranging them into a sequence so as to define a geometry volume to be simulated, in a manner analogous to building blocks (Figure 1).

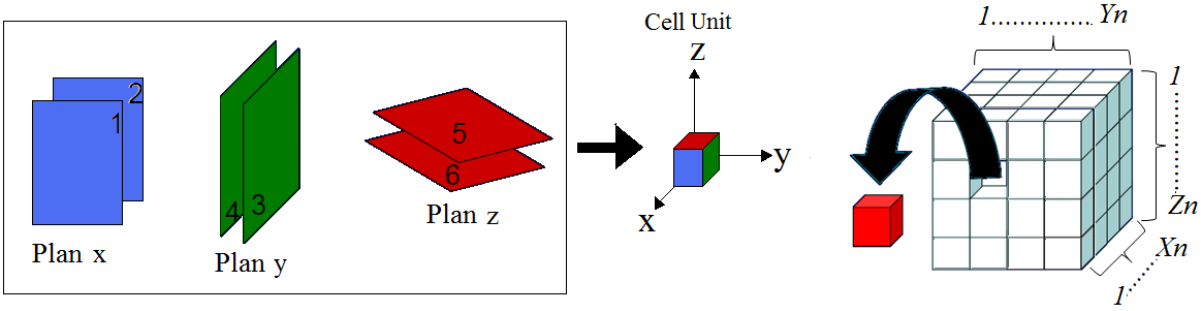

Figure 1. Geometric modeling, the intersection of the planes x, y and z in a CELL in the MCNP code, and it arrangement to modeling the sequence of the main block.

Each CELL unit has its composition and material specific, which can be altered for facilitate the modeling of the irregular and heterogeneous volumes. A CELL can be filled directly by a material defined in the code, resulting in homogeneous geometries, or the concept of the UNIVERSE. This concept is either a lattice or an arbitrary collection of cells. A single universe, described only once, can be designated to fill each of any number of cells in the geometry [5].

In this context, voxel phantoms are modeled by the association of resolutions images elements (pixels - picture element), with the UNIVERSE's concept. The arrangement of the CELL filled by the UNIVERSE model the structures of realistic human anatomy in the code, as shown in Figure 3.

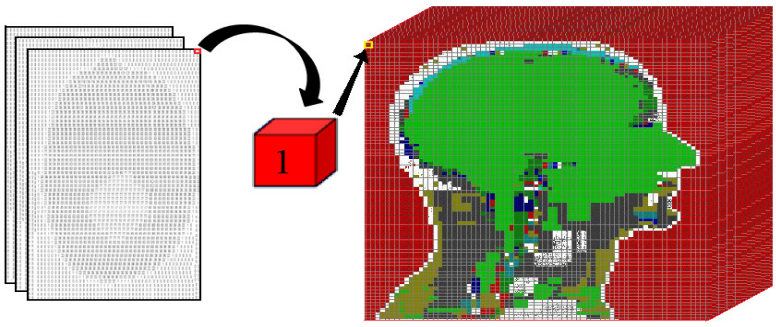

Figure 3. Pixels' array associated with the concept of UNIVERSE, which in turn fills the CELLS in an array, modeling the realistic human anatomy in the MCNP code.

***ISBN:* 978-85-99141-04-5**

In order to understand and evaluate the quality of this tool and the possible interference in the estimates of absorbed dose calculations, especially in body's thin regions, such as the skin, which are discriminated by the volume fraction of a unit CELL. This study proposes the modeling of a phantom using two different description methods in the code: the first using continuous surfaces pre-defined surfaces and; the second discretized structure by the repeating unit CELLS.

2. MATERIALS AND METHODS

TO verify the capacity and quality of Structure Repeated tool, as well as compares it with the representation of the continuous type in terms of absorbed dose estimates have been proposed the construction and dosimetric evaluation of a simple geometry to represent the human body.

The proposed geometry consists in a cylindrical disk of equivalent material to internal human tissue (ρ =1.05 g/cm³) surrounded by a cylindrical shell of material equivalent to human skin (ρ =1.09 g/cm³), surrounded by air. Initially it was proposed a study on a single slice of the body, resulting in four systems, each with 25.5 cm in diameter and 3.6 mm height, modeled by different methods of construction and discrimination of the skin.

The first system proposed was modeled by using of pre-defined cylindrical surfaces in the code, which were used to describe a continuous structure with a skin thickness of 1.5 mm (Figure 4A), according to the specifications of the ICRP 89 [9]. Throughout this study, it will be used the notation *Continuous Cylinder* (CC) to depict this representation.

The second system consists in the discrete representation of the first system, modeled using the segmentation and discrimination algorithm of the skin proposed by Antunes et al. [10]. In this representation, the skin region is located in all first voxels belonging to phantom's contour. Throughout this study, it will be used the notation *Simple Segmentation* (SS) to depict this model, as the skin thickness is 0.36 mm (same thickness of the voxel), according to Figure 4B.

The third and fourth systems were modeled identically to the second system, though with different representations of skin. The third cylinder discriminates the skin for a fraction of the voxel volume. This representation was accomplished by prior assessment of possible side neighbors of voxels, the N6(S)'s connections [11]. The skin is located only in the first 0.15 cm of voxel, which borders the air region (Figure 4C). Throughout this study, in this representation will be used the notation *Classified Segmentation* (CS) to depict this model [10].

In the fourth system, in the evaluation of the voxel connections, were increased the edge neighbors, which increases the number of the N18(S)'s connections [11], adding voxels and keeping skin thickness in 0.15 cm according to be specified by the ICRP 89 (Figure 4D). Throughout this study, in this representation will be used the notation *Diagonals Segmentation* (DS) to depict this model [10].

2011 International Nuclear Atlantic Conference - INAC 2011
Belo Horizonte, MG, Brazil, October 24-28, 2011
ASSOCIAÇÃO BRASILEIRA DE ENERGIA NUCLEAR - ABEN
***ISBN:* 978-85-99141-04-5**

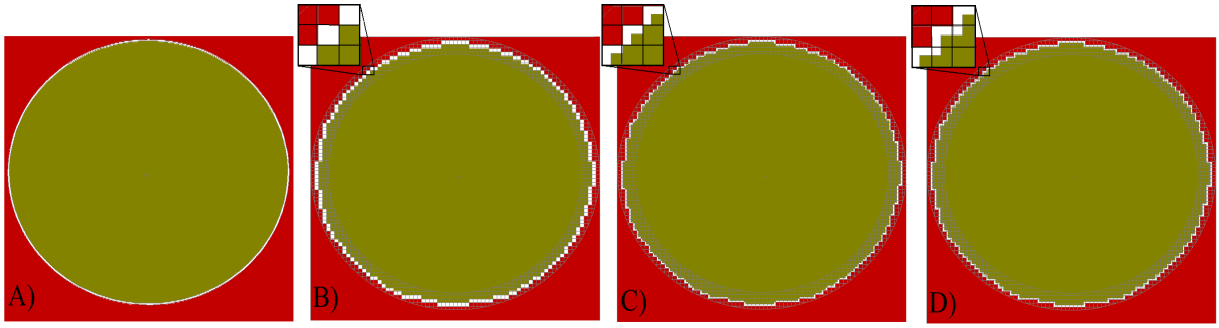

Figure 4. Cylinders consisting of representative material of soft tissue (green) and skin (white), immersed in air (red). A) *Continuous Cylinder* (CC). B) Discrete cylinder based on the SS model. C) CS model. D) DS model.

These cylinders have been rebuilt in a second step, modifying the height to 30 cm, seeking a poor representation, but proportional to human body.

3. RESULTS

The four models were simulated using a uniform and monoenergetic electron beam (6 MeV) on cylinders side. The *F8 *tally* was used for estimate of the energy deposited in the skin (shell cylindrical), with results in MeV. This tally is the standard card for dosimetry on MCNP code, once it quantifies for the deposited average energy in CELLS.

Table 1 shows the estimates of mass (*Skin mass*) and dosimetric evaluation (*Energy Deposited in the skin*) for the different systems and for a single slice. With their respective relative differences to continuous representation, in mass terms (*Rel. Dif. Mass*) and absorbed dose (*Dif. Rel. Dose*), this is determined through the ratio of the deposited energy and the mass. In this table was also included the term *FOM* (*Figure of Merit*), parameter associated to efficiency of simulation.

Table 1. Data of the geometric representations different and dosimetric evaluations in a cylindrical of 3.6 mm in height.

Cylinder (model)	*Skin mass (g)*	*Dif. Rel. Mass (%)*	*Energy Dep. Skin (10^{-1}) (MeV)*	*Absorbed dose (10^{-2}) (MeV/g)*	*Dif. Rel. Dose (%)*	*FOM (10^{+5})*
Continuous (CC) (Skin 1.5 mm)	4.70	-	4.349 ± 0.002	9.255 ± 0.003	-	2.8
Discrete (SS) (Skin 3.6 mm)	9.97	+112.4	8.221 ± 0.002	8.240 ± 0.002	-10.9	1.04
Discrete (CS) (Skin 1.5 mm)	5.24	+11.7	4.358 ± 0.002	8.318 ± 0.002	-10.1	1.04

ISBN: 978-85-99141-04-5

Discrete (DS) (Skin 1.5 mm)	5.99	+27.5	5.761 ± 0.002	9.637 ± 0.002	+4.1	1.04

As shown in Table 1, in mass terms, the discrete representation that best approximates the continuous representation is model-based in CS, with overestimation less than 12%. The other representations based on SS and DS models have larger discrepancies of values obtained in relation to the continuous geometric, with mass overestimated of 112 and 27%, respectively.

At deposited energy estimation, the SC model also shows the best result, with a difference of around 0.2% compared to the continuous cylinder. However, this better performance on the mass representation and deposited energy estimation is not observed in terms of skin absorbed dose, with differences of 10%.

Showing difference in the estimation of absorbed dose of 4%, the DS model supplant CS and SS models, compensating the mass over-representation by deposited energy overestimation.

In Table 1 is also observed parameter FOM, which evaluates obtained result's efficiency by simulation and its reliability. This greatness is indirectly proportional to multiplication of computational time by the square of relative uncertainty from average value. The higher value of FOM, greater is the results efficiency. Even for a simple system, as proposed, the modification of continuous cylinder representation to discrete cylinder causes an increase in the time computational of the order of 180%.

The values shown in Table 1 are for a single slice of the phantom, practically reducing the problem to two dimensions. A more realistic estimate is presented in Table 2, with 30 cm height cylinders, to which were added to the skin regions, not only on the sides, as well as on the lip of the cylinders.

Table 2. Data of the geometric representations different and dosimetric evaluations in a shell cylindrical of 30 cm in height.

Cylinder (model)	*Skin mass (g)*	*Dif. Rel. Mass (%)*	*Energy Dep. Skin (10^{-1}) (MeV)*	*Absorbed dose (10^{-2}) (MeV/g)*	*Dif. Rel. Dose (%)*	*FOM (10^{+3})*
Continuous (CC) (Skin 1.5 mm)	553.9	-	1.3834 ± 0.0003	2.4977 ± 0.0005	-	34.7
Discrete (SS) (Skin 3.6 mm)	1203.5	+ 117.3	2.5534 ± 0.0003	2.1216 ± 0.0002	- 15.1	10
Discrete (CS) (Skin 1.5 mm)	595.7	+ 7.5	1.3482 ± 0.0002	2.2633 ± 0.0002	- 9.4	10
Discrete (DS) (Skin 1.5 mm)	655.8	+ 18.4	1.8364 ± 0.0009	2.8005 ± 0.0002	+ 12.1	0.4

ISBN: **978-85-99141-04-5**

Table 2 also shows again an over-representation in the skin mass of discrete cylinders. However, the differences in values are reduced for CS and DS models, with skin thickness of 1.5 mm, especially for the ability to represent the lips, which are arranged parallel to one of the planes used in the formation of *Repeated Structure*. In this geometry, the best estimates of mass and deposited energy are presented by the CS model.

This model also provides the better results when comparing the differences in dose estimates and simulation performance. Particularly on this parameter is observed a sharp drop in obtaining results performance, with FOM reduction.

In this context, seeking to meet the best representation both in terms of mass and reliable dosimetric evaluation, the most appropriate model is Classified Segmentation (CS), which discriminates the skin by partial volume of the voxel and evaluates only the N6(S) connections neighboring.

4. CONCLUSIONS

The *Repeated Structure* is an powerful tool MCNP code, which allows more accurate representations of the geometry to be simulated and therefore is directly associated with the results reliability.

This study allowed an analysis of this tool, both in terms of mass and absorbed dose, once assessed the discretization level of the structures. In mass terms, as higher is the resolution more similar to the real representation; however, this representation is not reproduced in terms of absorbed dose. Since the discretization adds some simulation artifacts in the deposited energy.

After analyzing the relationship between mass and deposited energy, it was observed in this study that the representation more similar to the real is the representation that assess only the simple connections a voxel, N6(S) connections.

The geometries described in the code through the *Repeated Structure* tool require a computational time significantly greater than those described in pre-defined surfaces in the code. In addition to needing a more expressive computer memory. These factors are evaluated by the term FOM, for a single slice, as higher the discretization degree of a structure, the greater the value assigned to FOM.

The efficiency of a simulation is significantly changed, adding a third dimension to the structure, increasing the value about two orders of magnitude. This study assessed a simple geometry, however, to more complex and heterogeneous representations as the human body, this factor is strongly influenced by significantly reducing simulation's efficiency.

In this sense, a correct assessment of the best level of structure representation is extremely important to validate the use of the *Repeated Structure* tool, once the better representations in mass terms are directly associated with reduced efficiency of a simulation and validation the use of the tool and evaluations of body's thin structures.

ISBN: **978-85-99141-04-5**

REFERENCES

1. Bielajew, A. F., "*Fundamentals of the Monte Carlo Method for neutral and charged particle transport*", Michigan. U.S.A. (2001).
2. Salvat F., Fernandez-Varea J.M., Acosta E. and Sempau J., "*PENELOPE – A code system for Monte Carlo simulation of electron and photon transport*", Workshop Proceedings Issy-les-Moulineaux, France 5-7, Nuclear Energy Agency (2001).
3. Kawrakow I. and Rogers D. W. O., "The EGSnrc code system: Monte Carlo simulation of electron and photon transport National Research Council of Canada", Ottawa, Canada, PIRS-701, Webpage: http://www.irs.inms.nrc.ca/inms/irs/EGSnrc.html (2000).
4. Seltzer, S. M., "Electron-photon Monte Carlo calculations: the ETRAN code", *Appl. Radiat. Isot.,* **Vol. 42**, pp. 917-41 (1991).
5. Briesmeister, J. F., "*MCNP – A general Monte Carlo N-Particle transport code*", version 5, Los Alamos National Laboratory Report, LA-13709-M (2001).
6. Yoriyaz, H., Santos, A., Stabin, M. and Cabezas, R., "Absorbed fractions in a voxel-based phantom calculated with the MCNP-4B code", *Med. Phys.*, **Vol.27**, No. 7, pp. 1555-1562 (2000).
7. Spanier, J. and Gelbard, E.M., "*Monte Carlo principles and neutron transport problems*", Dover Publications (2008).
8. Jenkins T. M., Nelson W. R. and Rindi A., *"Monte Carlo transport of electrons and photons*", Ettore Majorana Science Series, Plenum Press, New York (1988).
9. ICRP - International Commission on Radiological Protection, "*Basic anatomical and physiological data for use in radiological protection: Reference Values 89*", ICRP Report nº 89, Pergamon Press, Oxford (2003).
10. Antunes, P.C.G., "*Reconstrução de Objetos Simuladores Segmentados Aplicáveis à Dosimetria de Pele*" Dissertação de Mestrado - Instituto de Pesquisas Energéticas e Nucleares - IPEN/CNEN-SP, São Paulo. Orientador: Paulo de Tarso Dalledone Siqueira (2010).
11. Gonzalez, R. C. and Woods, R. E., "*Digital image processing*", Second edition, Prentice Hall (2002).