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Additional Information

# Toolkit implementation to exchange phase-space files between IAEA and MCNP6 Monte Carlo code format

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## Toolkit implementation to exchange phase-space files between IAEA and MCNP6 Monte Carlo code format

Purpose: Some Monte Carlo simulation codes can read and write phase space files in IAEA format, which are used to characterize accelerators, brachytherapy seeds and other radiation sources. Moreover, as the format has been standardized, these files can be used with different simulation codes. However, MCNP6 has not still implemented this capability, which complicate the studies involving this kind of sources and the reproducibility of results among independent researchers. Therefore, the purpose of this work is to develop a tool to perform conversions between IAEA and MCNP6 phase space files formats, to be used for Monte Carlo simulations. Materials and Methods: This paper presents a toolkit written in C language that uses the IAEA libraries to convert phase space files between IAEA and MCNP6 format and vice versa. To test the functionality of the provided tool, a set of verification tests has been carried out. In addition, a linear accelerator treatment has been simulated with the PENELOPE library using the PenEasy framework, which is already capable to read and write IAEA phase space files, and MCNP6 using the developed tools. Results: Both codes show compatible depth dose curves and profiles in a water tank, demonstrating that the conversion tools work properly. Moreover, the phase space file formats have been converted from IAEA to MCNP6 format and back again to IAEA format, reproducing the very same results. Conclusion: The toolkit developed in this work offers MCNP6 scientific community an external and validated program able to convert phase space files in IAEA format to MCNP6 internal format and use them for Monte Carlo applications. Furthermore, the developed tools provide also the reverse conversion, which allow sharing MCNP6 results with users of other Monte Carlo codes. This capability in the MCNP6 ecosystem provides to the scientific community the ability not only to share radiation sources, but also to facilitate the reproducibility among different groups using different codes via the standard format specified by the IAEA.

Keywords: IAEA phsp format, phase space file, Monte Carlo simulations, MCNP

### Introduction

Monte Carlo (MC) methods for simulation of radiation transport through matter are used in several applications, for example to characterize detectors, to obtain absorbed

energy distributions in radiological protection field, dosimetry calculations, in medical physics, several processes in the industry, etc. Indeed, these methods have become increasingly used in medical physics in the last years, especially in radiotherapy treatments. An example of its application in the medical physics field, is the calculus of the absorbed dose distribution in patients undergoing treatments with beams emitted by a Linear Accelerator (LinAc) (Verhaegen et al. 2003, Rogers and Bagheri 2006). This kind of studies require a precise description of the accelerator geometry and material compositions to be able to characterize the outgoing radiation beam. Unfortunately, the simulation of the accelerator itself involves a huge computational time. However, treatments involving the same LinAc configuration use the same beam. Thus, saving the beam characteristics in a scoring surface, allows the simulation to be performed without repeating the beam simulation through the accelerator geometry, significantly speeding up the entire simulation process. This is done via the phase space (*phsp*) files, which register the necessary information to characterize the state of each particle reaching a scoring region, i.e., saves, at least, the energy, direction, position, statistical weight and particle type. Extra variables could be included also depending on the MC code. For instance, following the LinAc example, the scoring region is commonly located at the exit of the head (IAEA Nuclear Data Section 2006).

Although the capability to create *phsp* files is wide implemented in most MC codes, each one uses their own specific format, which limits compatibility and reproducibility between different codes. Aimed to solve this issue, the International Atomic Energy Agency (IAEA) has defined a standard *phsp* format which can be read and written using its libraries, which are freely offered. Using this format, the IAEA has created a public database (IAEA NAPC, 2020) of *phsp* files from linear accelerators used in external radiotherapy, by compiling existing data that have been properly validated. Also, this format is used by therapy unit manufacturers to provide the *phsp* information of a commercial device when this is required by hospitals or research groups for different purposes as calibrations, or dose estimation in radiotherapy planning. Considering that manufacturers information is usually subjected to strong confidential agreements, this approach greatly simplifies the procedures to be able to carry out studies on this type of device. Furthermore, as has been discussed, it also avoids the repetition of lengthy MC calculations performed already by others research groups and enhances reproducibility among different groups and codes providing a set of common data for several applications.

Due to the advantages that a standardized format offers, many general-purpose MC codes have implemented compatibility with IAEA *phsp* format. For example, it is the case of BEAMnrc/EGSnrc (Kawrakow, 2017), penEasy/PENELOPE (Salvat, 2009, Sempau et al., 2011), and Geant4 (Agostinelli et al., 2003, Cortés-Giraldo et al., 2012). Unfortunately, MCNP6 (Los Alamos Scientific Laboratory, 1979) does not have an implementation of the IAEA format recognition. Therefore, it is not possible to run phase spaces files written in this standard format in MCNP6 simulations, and neither allows to write *phsp* files generated with MCNP6 in this format. This fact limits both, the capability of MCNP6 users to reproduce the results of other researchers, and the reproducibility of MCNP6 results with other codes. Considering that the reproducibility has lately become a topic of interest for researchers and institutions worldwide (European Commission, 2016, Public Library of Science), is interesting to address this MCNP6 limitation. Moreover, in the specific case of medical physics, the results published in international protocols, such as the TRS-398 (IAEA, 2005), are calculated independently by several research groups, who use different MC codes, to stablish a consensus of the calculated data (Giménez-Alventosa et al., 2020). Therefore, the

capability to share phase space files between different codes could enhance the suitability of MCNP6 to be present in this kind of shared studies.

Aimed to address the mentioned limitations, this work presents the development of a freely distributed open-source library, written in C language, able to read *phsp* files provided in the IAEA format and convert them into the binary format used by the MCNP6, and vice versa. Therefore, it allows to use IAEA *phsp* files for MCNP6 simulations and share MCNP6 calculated *phsp* to be used by IAEA compatible applications and to be submitted to the IAEA database.

#### **Materials and methods**

In this section, the components used to develop the presented tools are described. These tools consist of two programs. The first one, is capable to convert from IAEA into MCNP6 *phsp* format and is named IAEA2MCNP. The second one, named MCNP2IAEA, performs the reverse conversion, i.e., from MCNP6 to IAEA format. Both use the IAEA provided library to be able to read and write its *phsp* format. The IAEA files with the routines and the corresponding documentation are available at the web site of the IAEA *phsp* project<sup>1</sup>. Take into account that both programs have been implemented for MCNP6.1 and MCNP6.2, which are, currently, the latest versions of MCNP6. As future versions of MCNP could involve changes on the *phsp* header or in its internal format, these tools should be revised and upgraded to ensure compatibility with the future versions of MCNP. In the remaining section, both, IAEA and MCNP6 *phsp* formats will be briefly described along with the considerations taken into account to perform the conversions. Then, the performed tests will be described.

<sup>&</sup>lt;sup>1</sup> <u>http://www-nds.iaea.org/phsp</u>

#### **Description of IAEA phsp format**

The IAEA *phsp* consist of two files. The first one is a binary file of extension ".IAEAphsp" (Capote, 2006), which registers the state of all particles that reach the scoring surface i.e., energy (E), in MeV, particle type (represented by a number associated with each of them: photon = 1, electron = 2, positron = 3, etc.), statistical weight (*wght*), the cartesian component of the position (x, y, z) in cm, the direction cosines of the linear momentum (u, v,w), some storage space for integer extra variables, as the incremental history number ( $n_{sat}$ ) among others. The second file is an ASCII file with extension ".IAEAheader". This one specifies the format and structure of the data or event generator code, such as the used byte order, the *phsp* size, etc.

An example of the *phsp* file is shown in the Table 1, where the "iaea2ascii" tool provided by the IAEA project has been used to covert the binary *phsp* to ASCII. In this table, PT refers to the particle type, and Ch refers to the charge of the particle.

Table 1. An example of the information in a phase space file in IAEA format (4 particles).

## Description of MCNP phsp format

MCNP6 code provides the capability to write and read *phsp* files with two input cards. The first card is the Surface Source Write (SSW), which is associated to a geometry surface defined in the input file. It is used to record the state of any particle that crosses the scoring surface. The second card, the Surface Source Read (SSR), is used to read the particle information stored in the surface source file and uses that information as a source in a subsequent MCNP6 simulation. More information of these cards can be found at MCNP User's Manual (Goorley, 2012), (Werner, 2017), (Werner, 2018). Nevertheless, no formal documentation of the MCNP *phsp* binary format exists, and its format has change between MCNP versions. Despite this, the internal format of the phsp files of the MCNP code for versions 6.1 and 6.2 has been exhaustively studied in this work, reaching the following conclusions. The phsp generated with MCNP6 is written in a single file which includes the header and the list of particle state variables. The header is organized in six sections and contains relevant information as the name and version of the code that wrote the surface source file, the date when the file was written, the number of simulation histories, or the number of tracks recorded in the source surface, among other variables. Fortunately, most of these fields, are only informative to the MCNP code and its values neither are mandatory nor affect the simulation results. Therefore, these information fields can be filled with default values allowing the MCNP6 to work properly. Following the header information, the particles data <mark>is</mark> found, containing a list of state variables of each particle. These ones are particle type, energy, cartesian components of the position, statistical weight, particle direction cosine with *X* and *Y* axis, the time of flight of the particle, the history number and the number of the surface where the *phsp* file was recorded.

#### **Conversion between IAEA and MCNP phsp format**

Due to the differences between IAEA and MCNP *phsp* formats, some considerations must be taken into account to perform the conversion tools.

Firstly, the IAEA format provides the three direction cosines (u, v, w), but MCNP write only two of them u and v. Nevertheless, as the direction is considered to be normalized to the unit i.e.,  $u^2+v^2+w^2=1$ , the w value is calculated

by the MCNP2IAEA tool to be written in the IAEA *phsp* file. However, as the sign of

*w* cannot be determined only with *u* and *v* information, in the MCNP format this sign is provided via the particle type. For instance, in MCNP6, the particle type number assigned to photons is "16". If the *Z* component of the photon direction is positive, the particle type in the *phsp* is set to "+16" but is assigned to "–16" otherwise. Using this information, the correct sign can be assigned to the calculated *w* variable. The inverse procedure is used in the conversion from IAEA to MCNP format.

Secondly, in the MCNP *phsp* particle list, the number of the scoring surface is a mandatory variable, which is not provided in the IAEA format. To solve this problem, the user must specify it as an argument in the execution of the IAEA2MCNP tool. Finally, the time of flight of each particle is written in the MCNP *phsp* format but not by the IAEA. Therefore, the time is set by default to zero when IAEA2MCNP tool is used

to convert between formats. Notice that it is a limitation of the IAEA format.

#### Verification tests

In this section, a set of verification tests have been carried out involving only file format conversions, i.e., with no interaction simulation. The first test of this section will check the conversion using *phsp* files of the IAEA database. Then, a second test has been defined to check the conversion from *phsp* files produced by MCNP6.

In the first test, to check the correct conversion between formats, a set of IAEA *phsp* files have been converted to the MCNP6 format and then, converted back to IAEA format. The *phsp* analysed in this section corresponds to the "Varian\_Clinac\_600C\_6MV\_10x10.IAEAheader" and "Varian\_Clinac\_600C\_6MV\_10x10.IAEAphsp", both downloaded from the web site of the IAEA *phsp* project<sup>2</sup>. The main characteristics of this *phsp* are summarized in the Table 2.

Table 2. Main characteristics of the phsp file used in the first verification with the aim to verify the correct conversion between formats.

To evaluate the equivalence between converted files, both *phsp* were analysed, i.e., the original IAEA *phsp* and the produced *phsp* after IAEA to MCNP6 conversion and MCNP6 to IAEA conversion. To perform the comparison the "iaea2ascii" utility provided by the IAEA has been used.

The second test has been designed to check the correct assignation of the sign in the Z direction component. In addition, this test will verify the correct reading and writing of the *phsp* files when the conversion tools has been used on MCNP6 generated *phsp*.

<sup>&</sup>lt;sup>2</sup> http://www-nds.iaea.org/phsp/photon/)

Moreover, the test will involve a different MC code to ensure the compatibility of the generated IAEA *phsp*. For this purpose, an MCNP6 simulation has been performed generating a *phsp* file, which conversion to IAEA format has been tested with penEasy. PenEasy has been chosen because it implements the capability to both, simulate and generate directly phase space file in the IAEA format. Therefore, penEasy allows an easy validation of both tools, IAEA2MCNP and MCNP2IAEA.

The set up of this test is shown in Figure 1 and described following. First, a I-131 photon source located at (0, 0, 0), aiming to + Y axis, was simulated with MCNP6 code with  $1 \cdot 10^7$  primary particles. This source consists of a cone that produces a circular field of  $r_1 = 5 cm$  at  $y_1 = 10 cm$ . Notice that this configuration will produce particles in positive and negative directions in both, Z and X axis. Therefore, this case tests the correct assignation of the sign in the **Z** direction component (w). At  $y_1$ , the *phsp*<sub>1</sub> is used in two simulations. The first one continues the simulation with another MCNP6 run using the  $phsp_1$  as source, simulating all the particles scored. For the second case, the  $phsp_1$  is converted to IAEA format and then, used as a source of a penEasy simulation. The simulations in both codes are equivalent, i.e., from  $y_1$  to  $y_2=20 cm$ , generating a field of  $r_2=10 cm$  at the last surface. Finally, a  $phsp_2$  is scored at  $y_2$  with both, the penEasy and MCNP6 simulations. In the first simulation, resulting  $phsp_2$  from penEasy run is obtained directly in IAEA format by the penEasy code and then is converted to ASCII using the mentioned "iaea2ascii" tool provided by the IAEA project. In the second simulation, the resulting *phsp*<sub>2</sub> from MCNP6 run is converted to IAEA using MCNP2IAEA tool and then to

ASCII with "iaea2ascii". Finally, both IAEA ASCII phsp<sub>2</sub> were compared <mark>and</mark> <mark>analysed</mark>. To isolate the problem of format conversion, an empty universe with void material has been simulated to not affect the particle tracking. Thus, differences in the physics implementation will not affect the final results. The *phsp* quadric surfaces are also assigned to void material. These simulations have been executed in SENUBIO ISIRYM research group's cluster, named Quasar, with a parallelized version of MCNP6 using the MPI standard with 26 processes. The 6.1 version for MCNP6 simulations has been used, and the penEasy version v2020-03-25, for penEasy/PENELOPE simulations. Figure 1. Set up diagram of the MCNP and penEasy/PENELOPE simulations of a conical source with two scoring surfaces defined.

#### **Complete tests**

In this section, a complete set of tests with simulations of a LinAc beam directed to a water tank has been performed. To verify both tools, MCNP6.1 and the latest version of penEasy/PENELOPE codes have been used. Following, the simulations performed are described, which have been done with an objective uncertainty of 3%.

#### IAEA2MCNP test

To test the IAEA2MCNP tool a *phsp* file of a 6 MeV photon beam issued by the medical linear accelerator Varian Clinac 600 C provided by the IAEA database was used. As the header of this *phsp* file indicates, the MC codes used for this LinAc geometry construction and the phase space file generation were PENELOPE 2008, penEasyLinac and penEasy v.2009 (Salvat, 2019), (Sempau et al., 2011).

The geometry model of the Clinac emitting a photon beam includes the tungsten target, primary collimator, flattening filter, ionization chamber, and the adjustable X and

*Y* jaws photon collimators. In this model, the gantry is vertically oriented (0 degrees). This *phsp*, was created with an electron monodirectional point source, generating a monoenergetic beam of 5.88 MeV, with  $2.3 \cdot 10^7$  original histories. The origin of the source is at z=0 cm upstream face of the target, and the central position of the target is located at x=0 cm, y=0 cm. The upper and lower jaws apertures have been configured to provide a field size of  $10 \times 10$  cm<sup>2</sup> at a source to surface distance (SSD) equal to 90 cm. Finally, the *z* axis direction is parallel to the beam direction, pointing downstream and the *phsp* scoring plane is located at z=66.8 cm from the source.

The IAEA2MCNP tool developed in this work, is used to convert the described *phsp* file from the IAEA format to MCNP6 binary format. A simulation with MCNP6 has been performed using the converted *phsp* as a source with  $1.15 \cdot 10^9$  number of particles. This one, simulates the particle transport from the *phsp* source surface, at *z*=66.8 cm, to a liquid water tank of 40 cm size in each axis, centered in (*x*, *y*) = (0,0). The surface of the water tank is located at *z*=90 cm, i.e., SSD of 90 cm. To obtain the depth dose and profiles curves along the water tank, the MCNP6 tally named "TMESH Type 3" is used. This tally returns the total energy deposited in each cell of a grid overlaid on top of the problem geometry, normalized by history. In this case, a rectangular mesh is chosen. Each of these cells is a voxel with size of  $0.2 \times 0.2 \times 0.2 \times 0.2$  cm<sup>3</sup>. The absorbed energy values are directly converted to dose using the water density (in g/cm<sup>3</sup>).

To validate the obtained results with the MCNP6 code, the same IAEA *phsp* described before is used as a source in a penEasy/PENELOPE simulation, reproducing identical

conditions (SSD, water tank dimensions, number of particles, etc). The dose depth and profiles curves has been obtained, with the same voxel size, using the Spatial Dose Distribution tally, which returns the absorbed dose per history in each voxel.

#### MCNP2IAEA test

In this case, to validate the MCNP2IAEA capabilities, a detailed simulation of a Varian Clinac 2100 C model, emitting a 6 MeV photon beam is performed. The geometry of the LinAc has been accurately modelled and it is shown in the Figure 2, including all the head accelerator components. This detailed geometry has been created thanks to the blueprints transferred to ISIRYM research group under a confidential agreement with Varian for research purposes. The geometry has been generated using 3D Modeling Software for Engineering ANSYS SpaceClaim, and the solid model has been meshed with Abaqus/CAE (Abaqus, 2014). Meshed geometries present the advantage of a higher accuracy in the geometry modelling. The unstructured grid imported from Abaqus/CAE is used as the input file geometry for the MCNP6 simulation, which enables the use of different cells, allowing the construction of complex geometries and optimizing the number of cells used. The geometry model has been previously validated with experimental results (Morató et al., 2017).

Figure 2. Three-dimensional geometry model of the Varian Clinac 2100 C used for 6 MeV photon beam and 10x10 cm<sup>2</sup> field size. Geometry modelled using SpaceClaim.

A simulation of the described LinAc configuration has been performed with the corresponding photon spectra obtained from (Sheikh-Bagheri et al., 2002), with the gantry vertically oriented. MCNP6 allows to simulate a wide type of particles

depending on the problem. To specify the particle types to be simulated, MCNP6 includes a field named "mode" in the configuration file. Among the available modes, in this case, the "mode P E" has been selected to enable the tracking of photons (P) and electrons (E). The number of particles is set to  $1 \cdot 10^9$ , achieving standard deviations below 3%. The apertures set for *X* and *Y* jaws generate a field size of 10 x 10 cm<sup>2</sup> at an SSD of 100 cm. The particle beam has been aligned parallel to the *z* axis, pointing downstream, along the accelerator head. Finally, the particles at the exit of the LinAc are stored in a surface source in a *phsp* file.

The resulting *phsp* file is used as a source for the second simulations step. Therefore, a simulation with the penEasy/PENELOPE code has been performed with the converted MCNP6 *phsp* to IAEA *phsp* format. As performed with IAEA2MCNP tool tests, the simulation consists of particle transport from the source surface to a water liquid tank with 40 cm size in each axis, but, located at an SSD=100 cm. Dose results from depth dose and profiles curves along the water tank are obtained using the Spatial Dose Distribution tally with voxel size of 0.2 x 0.2 x 0.2 cm<sup>3</sup>. To validate obtained results with penEasy/PENELOPE code, an analogous simulation running directly the *phsp* with MCNP6 code was performed, using the same voxel size for dose results.

#### Results

In this section, the results of both verification and complete tests described in the previous sections are discussed. Notice that for complete tests, dose curves are presented in units of eV/g per history, where a history refers to a primary particle entering in the LinAc head accelerator and all its secondary particles.

## **Results for verification tests**

For the first verification test, the IAEA phsp files, which main characteristics are

described in Table 2, have been converted to MCNP format and converted back to IAEA format, and the resulting files are evaluated. Both files produce the very same distribution for each variable of the *phsp*, since the differences between each parameter of the *phsp* file are zero. For the sake of brevity, Figure 3 shows the histograms of energy, x and u distributions for photons and energy, y and v for electrons. However, all the *phsp* parameters are compared between original and converted files showing identical results. These comparisons shown that the original file and the converted to MCNP and converted again to IAEA format are identical.

Figure 3. Histogram of *phsp* parameters distributions between the original set of files of IAEA *phsp* downloaded from the IAEA database and the same converted to MCNP and back to the IAEA format. Energy, x and u distributions are shown for photons (left) while energy, y and v distribution are shown for electrons (right).

The second verification test which consists of a simulation of a I-131 photon conical source with two scoring surfaces was also analysed. In this case both IAEA ASCII **phsp**<sub>2</sub> obtained with penEasy/PENELOPE and MCNP respectively, were compared.

Figure 4 shows the equivalence between the energy spectrum while Figure 5 shows the comparison between the particle position distribution for penEasy/PENELOPE (left) and MCNP6.1 (middle). In this case the field at  $y_2$  is shown with the corresponding radius ( $r_2$ ). Finally, Figure 5 right, shows the voxel-to-voxel relative differences between particle distribution of both codes, presented in percentage. As it is shown, both distributions are completely equivalent. In fact, the differences of the 99% of the voxels are zero and the other 1% is within the ±0.5%. These minor differences have been attributed to rounding differences between MCNP6 and penEasy codes.

Figure 4. Energy distribution corresponding to both MCNP and penEasy/PENELOPE

#### simulations at *phsp*<sub>2</sub> surface.

Figure 5. Particle distribution for penEasy/PENELOPE simulation scored at phsp2 surface (left), particle distribution for MCNP6.1 run scored at the same surface (middle), and the ratio between distribution of both codes (right).

#### **Results for IAEA2MCNP tool**

Figure 6 and Figure 7 show the depth and profile dose distributions, respectively, obtained using the phase space file of Varian Clinac 600 C provided by the IAEA database.

For the sake of clarity, the dose values of these figures are shown using empty symbols for penEasy/PENELOPE and with filled symbols for MCNP6. In both cases, the represented error bars correspond to two standard deviation ( $2\sigma$ ). These error values are directly provided by the simulation code. To ensure that distributions simulated with both codes are compatible, a test over each depth point has been done. For instance, Figure 8 left presents the quotient, point by point, of both depth dose distributions showing the relative deviation between them. In this graph, the error bars represent on standard deviation of the quotient. As can be seen, all points are well distributed around the 1, as expected due the statistical uncertainties. Moreover, in the Figure 8 right, the distance in standard deviations, compared again point by point between both codes, has been histogrammed. This one show that the 97.5% of differences are within  $2\sigma$  and all of them are within  $3\sigma$ , demonstrating the compatibility between MCNP6 and penEasy/PENELOPE calculated distributions. This analysis has been repeated also for dose profile distributions at different z values showing an equivalent behaviour.

To compare the whole dose distribution and not only a 1D set of profiles and depth dose a 3D gamma evaluation (Low et al., 1998) has been done with 1%/1mm tolerance between MCNP6 and penEasy/PENELOPE distributions. The percentage of voxels with γ less than 0.05 was 98.3% and all of them are below 0.23. It is concluded that no dosimetric differences exist. Moreover, Figure 9 presents the γ values for the YZ plane at X=0 cm showing the γ distribution along the water tank depth.

Figure 6. Depth dose curve along the *z* axis of a water tank at SSD=90 cm obtained with penEasy/PENELOPE (empty symbols and error bars of  $2\sigma$ ) and MCNP6 (filled symbols and error bars of  $2\sigma$ ) after phase space file conversion using IAEA2MCNP tool.

Figure 7. Lateral profiles along *y* axis at different water tank depths, obtained with penEasy/PENELOPE (empty symbols and error bars of  $2\sigma$ ) and MCNP6 (filled symbols and error bars of  $2\sigma$ ) after phase space file conversion using IAEA2MCNP tool.

Figure 8. Ratio between penEasy and MCNP6 dose values of the depth dose distribution (left), and residual values from the penEasy and MCNP6 depth dose curves (right).

Figure 9. Gamma values for the YZ plane at X=0 cm showing the γ distribution along the water tank depth.

#### **Results for MCNP2IAEA tool**

The results obtained for depth and profiles dose curves using the phase space file generated with MCNP6 of a Varian Clinac 2100 C geometry, are shown in Figure 10 and Figure 11 respectively. To be consistent with the results of the previous section, in these figures, empty symbols are used for penEasy/PENELOPE dose values and filled symbols for MCNP6. The  $2\sigma$  for these values has been calculated, showing the corresponding error bars at Figures 10 and 11. Moreover, a study of the residuals and 3D y evaluation, as done in the previous test, shows the same behavior between MCNP6

and penEasy/PENELOPE distributions as the performed in the Figure 8 and Figure 9 respectively. Therefore, this study will not be discussed again in the current test.

Figure 10. Depth dose curve along the *z* axis of a water tank at SSD=100 cm obtained with penEasy/PENELOPE (empty symbols and error bars of  $2\sigma$ ) and MCNP6 (filled symbols and error bars of  $2\sigma$ ) after phase space file conversion using MCNP2IAEA tool.

Figure 11. Lateral profiles along y axis at different water tank depths, obtained with penEasy/PENELOPE (empty symbols and error bars of  $2\sigma$ ) and MCNP6 (filled symbols, with error bars of  $2\sigma$ ) after phase space file conversion using MCNP2IAEA tool.

#### Conclusions

MCNP6 Monte Carlo code has still not implemented the capability to read and write phase space files using the IAEA format. Therefore MCNP6 users cannot use *phsp* files from IAEA database or other files in this format. The lack of this capability in the MCNP6 code, makes difficult to compare results with other research groups, limiting the reproducibility capabilities of MCNP6 and its suitability to be used on comparative studies. Moreover, as most manufacturers provide their spectra using the IAEA format, to avoid sharing details on the hardware geometry and materials due to confidential agreements, MCNP6 was not capable to perform studies with this kind of sources. Nevertheless, the tool developed in this work solves these problems, offering to the MCNP6 scientific community an external program able to read *phsp* files in IAEA format and write it in the internal binary MCNP6 format. Furthermore, the developed tools provide also the reverse conversion, write in IAEA format a *phsp* file generated with an MCNP6 run. Both tools have been validated in this work showing a perfect agreement between original and converted *phsp* files in all cases. Although the verifications have been done against radiotherapy applications with linear accelerators, both tools are application independent, and can be used with no restriction on any IAEA or MCNP6 *phsp* file. Also, a complete simulation has been compared against the penEasy/PENELOPE code, which already implements the capability to use the IAEA *phsp*, showing, once again, a perfect agreement.

In addition, the provided tools require no user knowledge about the MCNP6 nor IAEA *phsp* format, being easy to use. Furthermore, they only require the file names as input parameters. Aditionally, the MCNP2IAEA tool will allow to increment the IAEA data base with *phsp* generated with MCNP6 MC code, as well as use MCNP6 generated *phsp* with other codes for comparing and validating results.

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#### **Declaration of interest**

The authors report no conflicts of interest. The authors are only responsible for the content of the paper.

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