The Monte Carlo simulation of a Package formed by the combination of three scintillators: Brillance380, Brillance350, and Prelude420.

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I- Introduction

The objective of this work is to study the behaviour of a package formed by the combination of three scintillators, Brilliance 380 ($LaBr_3$; Ce), Brilliance 350 ($LaCl_3$; Ce), and Prelude 420 ($Li_{1.8}Y_{0.5}SiO_5$; Ce), for photons and protons, using different geometries, different energies and different source-detector distances, by the use of the MCNP code (**M**onte **C**arlo **N**- **P**article computer code).

II- The MCNP code

MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, also proton (new version: MCNPX), or coupled neutron/photon/electron/proton transport. The code treats an arbitrary three-dimensional configuration of materials in geometric cell bounded by first – and second – degree surfaces and fourth – degree elliptical tori. The code accounts for incoherent and coherent scattering, the possibility of fluorescent emission after photoelectric absorption, and absorption in electron – positron pair production. Electron/positron transport processes account for angular deflection through multiple coulomb scattering, collision energy loss with optional straggling, and the production of secondary particles including K X-rays, knock-on and Auger electrons, Bremsthralung, and annihilation at rest. Photonuclear physics is available for a limited number of isotopes.

The photon energy regime is from 1 keV to 100GeV, the electron energy regime is from 1 keV to 1GeV, and the proton energy regime is from 1 keV to 150MeV (new version: MCNPX).

The user creates an input file that is subsequently read by MCNP. This file contains information about the problem in areas such as:
- The geometry specification,
- The description of materials and selection of the cross section evaluations,
- The location characteristics of photon, proton, or electron source,
- The type of answers or tally desired, and
- Any variance reduction techniques used to improve the efficiency.

II-1 MCNP Geometry

The materials in geometric cells bounded by first- and second-degree surfaces and fourth-degree elliptical tori. The cells are defined by the intersections, unions, and complements of the regions bounded by the surfaces. Surfaces are defined by supplying coefficients to the analytic surface equations or, for certain types of surfaces, known points on the surfaces.

II- 2 Surface cards

The surface card contains: *j   a   list,*   where
- j = surface number: $1 \leq j \leq 99999$, asterisk: reflecting surface or plus:white boundary.
- a = surface mnemonic, (plane, sphere, cylinder, etc.).
- List = numbers that describe the surface like; dimension, radius, etc., in cm.

In the example above, the number of the surface is 1. The mnemonic cz defines an infinite cylinder centred on the z-axis, with a radius of 20.0 cm. The $ terminates data entry and everything that follows, <u>infinite z cylinder</u>, is interpreted as a comment, providing the user with more detail.

Example 1:

1	cz	20.0 $ infinite z cylinder

Figure 1: Surface card data

II- 3 Cell cards

Cells are used to define the shape and material content of physical space. The specific format for a cell card is: j   m   d   geom   param

   j = Cell number, starting in column 5.

   m = Material number, (zero if cell is void).

   d = Cell material density:

   No entry if cell is a void.

   Positive entry = atom density (atom/b-cm).

   Negative entry= mass density (g/cc).

   geom = list of all signed surface numbers and Boolean operators that specify a cell.

   param = Optional specification of the cell parameters.

The cell number, j, is an integer from 1 to 99999. The material number, m, is also an integer from 1 to 99999 that determines what material is present in the cell. The composition of a specific material is defined in the data card section. A positive entry for the cell material density, d, indicates an atomic density in *atoms per barn-centimetre.* A negative entry indicates a mass density in *grams per cubic centimetre*. The geometry specification, geom, consists of signed surface numbers combined with Boolean operators to describe how regions of space are bounded by those surfaces. Surfaces are the geometric shapes used to form the boundaries of the problem being modelled. The optional param feature allows cell parameters to be specified on the cell card line instead of in the data card section.

Example 2:

C cell card
1   1   -0.9999   -1   imp: p=1
C surface card
1   so   20.0 $ sphere centred at the origin 0, 0, 0, and 20.0 is a sphere radius.

This example is a bare sphere of water. As shown, the material density is -0.9999, because 0.9999 is negative the units are g/cc. The next entry, -1 indicates that cell 1 inside the surface number 1 (inside the sphere), is all space having a negative sense with respect to surface 1. The imp: p=1, says this cell has an importance (imp) for photons (: p) of 1 (the imp card has a role to help particles move more easily to important regions of the geometry. The importance of a cell is used to terminate the particle's history if the importance is zero). A blank line delimiter concludes the cell card section.
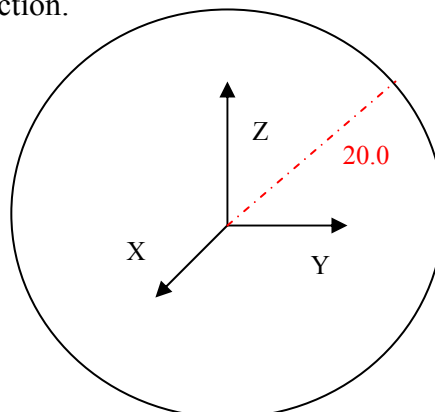

Figure 3: a bare sphere of water.

II- 4 Data cards

All MCNP input cards other than those for cells and surfaces are entered after the blank card delimiter following the surface card block. The mnemonic must begin within the first five columns. These cards fall into the following categories:

1- Problem type (MODE) Card : photon mode, electron mode, proton mode, or coupled photon/electron mode.
2- Source Specification.
3- Material specification.
4- Tally specification.

❖ **Problem type (Mode) card :**

Form   Mode x_1 …. x_i

x_1 = h proton mode transport.

P photon mode transport.

E electron mode transport.

❖ **Source Specification:**
❖

The source and type of radiation particles for an MCNP problem are specified by the SDEF command. The SDEF command has many variables or parameters that are used to define all the characteristics of all sources in the problem. The SDEF command with its many variables is one of the more complex MCNP commands and is capable of producing an incredible variety of sources — all with a single SDEF command. And only one SDEF card is allowed in an input file.

The source has to define the values of the following MCNP variables for each particle it produces:

ERG   the energy of the particle (MeV).
TME   the time when the particle started (shakes)
UUU, VVV, WWW   the direction of the flight of the particle
XXX, YYY, ZZZ   the position of the particle
IPT   the type of the particle
WGT   the statistical weight of the particle
ICL   the cell where the particle started
JSU   the surface where the particle started, or zero if the   starting point is not on any surface

❖ **Material Specification:**

Specification of materials filling the various cells in an MCNP calculation involves the following elements: (a) defining a unique material number, (b) the elemental (or isotopic) composition, and (c) the cross section compilations to be used. Note that density is not specified here. Instead, density is specified on the cell definition card.

This permits one material to appear at different densities in different cells. Suppose that the first material to be identified in problem input is (light) water and that only gamma-ray transport is of interest. Comment cards (cards beginning with C or c) may be used for narrative descriptions. In the following card images, the designation M1 refers to material 1. For a compound, normalized atomic fractions may be used.

Example 3:

```
c ---------------------------------------------------------------------
c WATER for gamma-ray transport (by atom fraction)
c ---------------------------------------------------------------------
M1 1000      2          $ elemental H and atomic abundance
   8000      1          $ elemental O and atomic abundance
```

Figure 4: Material card with atom fraction

The designations 1000 and 8000 identify elemental hydrogen, atomic number $Z = 1$, and elemental oxygen ($Z = 8$). The three zeros in each designation are place holders for the atomic mass number, which would be required to identify specific isotopes of the element. For compounds or mixtures, composition may alternatively be specified by mass fraction, indicated by a minus sign, as follows:

Example 4:

```
c ---------------------------------------------------------------------
c WATER for gamma-ray transport (by mass fraction)
c ---------------------------------------------------------------------
M1 1000     - 0.11190     $ elemental H and atomic abundance
   8000     - 0.88810     $ elemental O and atomic abundance
```

Figure 5: Material card with mass fraction

❖ **Tally specification**

Details of specifying tallies using tally cards and tally modification cards are given in the next paragraph. A summary of available tallies in MCNP5 is given below.

Table 1: Types of tallies available in MCNP. The type of particle tallies is denoted by *pl*.

Mneumonic	Tally Type	particles *pl*	Fn Units	*Fn Units
F1:*pl*	surface current	N or P or N,P or E	#	MeV
F2:*pl*	average surface flux	N or P or N,P or E	$\#/cm^2$	MeV/cm^2
F4:*pl*	average flux in a cell	N or P or N,P or E	$\#/cm^2$	MeV/cm^2
FMESH4:*pl*	track-length tally over 3D mesh	N or P or E	$\#/cm^2$	MeV/cm^2
F5a:*pl*	flux at a point or ring	N or P	$\#/cm^2$	MeV/cm^2
FIP5:*pl*	pin-hole flux image	N or P	$\#/cm^2$	MeV/cm^2
FIR5:*pl*	planar radiograph flux image	N or P	$\#/cm^2$	MeV/cm^2
FIC5:*pl*	cylindrical radiograph flux image	N or P	$\#/cm^2$	MeV/cm^2
F6:*pl*	energy deposition	N or P or N,P	MeV/g	jerks/g
F7:*pl*	fission energy deposition in a cell	N	MeV/g	jerks/g
F8:*pl*	pulse height distribution in a cell	P or E or P,E	pulses	MeV

III- Physical signification of Tallies:

The most frequently used tallies are current at a surface (F1), average flux at a surface (F2), and flux averaged over a cell (F4), and pulse height distribution in a cell (F8).

III- 1 The Surface Current Tally (type F1)

Each time a particle crosses the specified surface; its weight is added to the tally, and the sum of the weights is reported as the F1 tally in the MCNP output. Note that there is no division by surface area A. Nor is there a distinction between directions of surface crossing. When used with problem geometry voided (zero density), the tally is useful for verifying conservation of energy and conservation of number of particles. Technically, if $\mathbf{J}(\mathbf{r},E,\mathbf{\Omega}) \equiv \mathbf{\Omega}\Phi(\mathbf{r},E,\mathbf{\Omega})$ were the energy and angular distribution of the flow (current vector) as a function of position, the F1 tallies would measure.

$$\text{F1} = \int_A dA \int_E dE \int_{4\pi} d\Omega \, \mathbf{n}\bullet\mathbf{J}(\mathbf{r}_s, E, \mathbf{\Omega})$$

$$^*\text{F1} = \int_A dA \int_E dE \int_{4\pi} d\Omega \, E \, \mathbf{n}\bullet\mathbf{J}(\mathbf{r}_s, E, \mathbf{\Omega})$$

Where $\mathbf{n}$ is the outward normal to the surface at $\mathbf{r}s$.

III- 2 The Average Surface Flux Tally (type F2)

Suppose a particle of weight W crosses a surface, making angle θ with a normal to the surface. This particle makes a contribution $W|\sec\theta|/A$ to the flux (fluency) at the surface. The sum of the contributions is reported as the F2 tally in the MCNP output. Technically, if $\Phi(\mathbf{r}, E, \mathbf{\Omega})$ were the energy and angular distribution of the fluency as a function of position, the F2 tallies would measure.

$$\text{F2} = \frac{1}{A} \int_A dA \int_E dE \int_{4\pi} d\Omega \, \Phi(\mathbf{r}_s, E, \mathbf{\Omega})$$

$$^*\text{F2} = \frac{1}{A} \int_A dA \int_E dE \int_{4\pi} d\Omega \, E \, \Phi(\mathbf{r}_s, E, \mathbf{\Omega})$$

III- 3 The Average Cell Flux Tally (type F4)

Suppose a particle of weight W and energy E makes a track-length (segment) T within a specified cell of volume V. This segment makes a contribution WT/V to the flux (fluency) in the cell. The sum of the contributions is reported as the F4 tally in the MCNP output. Technically, if $\Phi(\mathbf{r}, E, \mathbf{\Omega})$ were the energy and angular distribution of the fluency as a function of position, the F4 tallies would measure.

$$F4 = \frac{1}{V} \int_V dV \int_E dE \int_{4\pi} d\Omega \, \Phi(\mathbf{r}, E, \mathbf{\Omega})$$

$$*F4 = \frac{1}{V} \int_V dV \int_E dE \int_{4\pi} d\Omega \, E \, \Phi(\mathbf{r}, E, \mathbf{\Omega})$$

III- 4 Pulse Height Tally (F8) Weight

The pulse height tally provides the energy distribution of pulses created in a cell that models a physical detector. It also can provide the energy deposition in a cell. Although the entries on the F8 card are cells, this is not a track length cell tally. F8 tallies are made at source points and at surface crossings. The pulse height tally is analogous to a physical detector. The F8 energy bins correspond to the total energy deposited in a detector in the specified channels by each physical particle (history). All the other MCNP tallies record the energy of a scoring track in the energy bin.

In an experimental configuration, suppose a source emits 100 photons at 10 MeV, and ten of these get to the detector cell. Further, suppose that the first photon (and any of its progeny created in the cell) deposits 1 keV in the detector before escaping, the second deposits 2 keV, and so on up to the tenth photon which deposits 10 keV. Then the pulse height measurement at the detector would be one pulse in the 1 keV energy bin, 1 pulse in the 2 keV energy bin, and so on up to 1 pulse in the 10 keV bin.

In the analogous MCNP pulse height tally, the source cell is credited with the energy times the weight of the source particle. When a particle crosses a surface, the energy times the weight of the particle is subtracted from the account of the cell that it is leaving and is added to the account of the cell that it is entering. The energy is the kinetic energy of the particle plus $2m_oc2 = 1.022016$ MeV, if the particle is a positron. At the end of the history, the account in each tally cell is divided by the source weight. The resulting energy determines which energy bin the score is put in. The value of the score is the source weight for an F8 tally and the source weight times the energy in the account for a $*$F8 tally. The value of the score is zero if no track entered the cell during the history. The pulse height tally depends on sampling the joint density of all particles exiting a collision event.

Another aspect of the pulse height tally that is different from other MCNP tallies is that F8:P, F8:E and F8:P,E are all equivalent. All the energy from both photons and electrons, if present, will be deposited in the cell, no matter which tally is specified.

When the pulse height tally is used with energy bins, care must be taken because of negative scores from non-analogue processes and zero scores caused by particles passing through the pulse height cell without depositing energy. In some codes, like the Integrated TIGER Series, these events cause large contributions to the lowest energy bin pulse height score. In other codes no contribution is made. MCNP compromises by counting these events in a zero bin and an epsilon bin so that these scores can be segregated out. It is recommended that your energy binning for an F8 tally be something like

E8 0 1.e-5 1. 2. 3. 4. 5…

Knock-on electrons in MCNP are non-analogue in that the energy loss is included in the multiple scattering energy loss rates rather than subtracted out at each knock-on event. Thus knock-on events can cause negative energy pulse height scores. These scores will be caught in the 0 energy bin. If they are a large fraction of the total F8 tally, then the tally is invalid because of non-analogue events. Another situation is differentiating zero contributions from

particles not entering the cell and particles entering the cell but not depositing any energy. These are differentiated in MCNP by causing an arbitrary 1.e-12 energy loss for particles just passing through the cell. These will appear in the 0-epsilon bin.

IV- MCNP simulation

In this work we have simulated, using MCNP computer code, a package formed by the combination of the following three scintillators:

Brillance 380 (LaBr3: Ce) built up by 9 crystals of $10(or15)*10*(or\ 15)*20*(or\ 30)$ mm^3.

Brillance 350 (LaCl3: Ce) built up by 9 crystals of $10(or15)*10*(or\ 15)*30*(or\ 60)$ mm^3.

Prelude 420 (Li1.2Y0.8SiO5: Ce) built up by 9 crystals of $10(or15)*10*(or\ 15)*30*(or\ 60)$ mm^3.

The crystals are separated by 0.3 mm of "Teflon".

This package is subjected to a mono-energetic point source (collimated into a cone of directions), with the following energies:

For photons: 5, 10, 25, and 30 MeV.

For protons: 10, 50, and 100 MeV.

The source detectors distances are 25, 30, 35, and 40 cm.

The combination of all the possibilities gives us a number of 512 input files to be treated by the MCNP computer code, which needs a no-negligible time of execution.

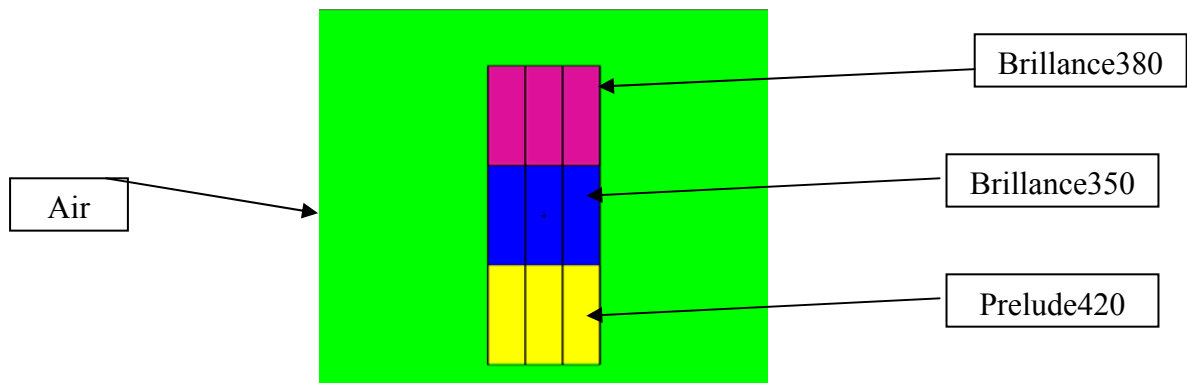The figures above show the package's geometry simulated with MCNP code.

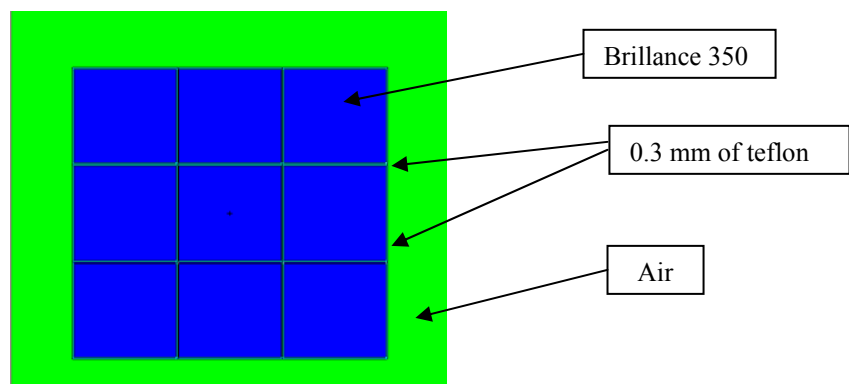Figure 6: Geometry simulated by MCNP in the XZ plane.

Figure 7: Geometry simulated by MCNP in the XY plane at (0, 0, 0).

V- Acknowledgement.