Development and Validation of a Geant4 Radiation Shielding Simulation Framework

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This paper details the development of a Monte-Carlo radiation shielding simulation framework using the C++ toolbox Geant4 for the CBETA accelerator. A scorer for equivalent dose, the primary quantity of concern, was developed and benchmarked against MCNP, showing good agreement. Radiation shielding simulations were performed in seven locations, measuring the gamma and neutron equivalent dose. The radiation maps are similar to MCNP but higher than physical measurements, calling for the addition of more objects in the simulations.

I. INTRODUCTION TO GEANT4

Geant4 ('**Ge**ometry **an**d **T**racking') is a C++ Monte-Carlo simulation toolkit developed by the Geant4 Collaboration under CERN and is used to describe interactions between particles and matter[1]. It has been shown, through significant benchmarking against physical experiments and other software, to be remarkably accurate at simulating interactions between particles and matter[2, 3]. Currently, Geant4 is being used on worldwide projects such as ATLAS, CMS, Muon g-2, and ILC[4], largely due to being accurate, open-source, and written in a modern language.

This openness and modernity is striking when compared to other Monte-Carlo simulation toolkits such as the Fortran toolkit MCNP (**M**onte-**C**arlo **N**-**P**article code), which is restricted in acquisition and use by the US government. Despite barriers in the use of MCNP and having been written in an antiquated language, MCNP is still considered industry-standard for many fields, including radiation shielding. This paper details the development and validation of a radiation shielding simulation framework in Geant4 aimed at flexibility and ease of simulations with the goal of replacing MCNP scripts.

II. INTRODUCTION TO RADIATION SAFETY

Whenever a high energy particle travels through a human body, there is a probability of interaction and damage in the form of cancer[5], acute radiation syndrome[6], or other sickness. Such damage is markedly biological, requiring experiments to accurately understand the danger of radiation. While basic physical quantities such as *dose deposit* (energy deposited per unit mass) can give a sense of dangers like acute damage[6], they fail to represent the risks for cumulative damage and the United States Nuclear Regulatory Commission (US NRC) has determined that cumulative damage is an important concern.

For example, the danger of 1 rad dose deposit from neutrons is often much worse than 1 rad dose from electrons since neutrons are more penetrating than electrons and they can induce radioactivity in the surroundings[7, 8] whereas electrons cannot. Furthermore, heavy particles such as alpha particles and protons are often less penetrating than lighter particles, and thus more likely to only damage skin, not sensitive organs. The wide variance in danger of each radiation (whether it is ionizing or not, how piercing it is, etc.) necessitates experiments in order to understand the danger of radiation.

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III. GEANT4 SIMULATIONS

In order to get a sense of cumulative radiological safety, the quantity equivalent dose is used, as recommended by the US NRC. With some modification, Geant4 can be used to measure this quantity via Monte-Carlo simulations. These simulations work via assigning each possible action a particle can undertake a probability, semi-randomly choosing an action, and then repeating the process until the particle has too little energy or exits the world. Doing this for many ($\sim$10 million) particles and averaging results gives a sense of the 'average' particle.

A. Physics Lists

The physics of the simulation is specified through *physics lists*, specifications on what actions particles can take (Bremsstrahlung radiation, neutron generation, etc.), probabilities of the actions, and how actions are taken. Geant4 provides a collection of 18 reference physics lists for different particles and energy ranges.

As this paper primarily concerns scattering relatively low energy particles (maximum energy primary is 150 MeV), the Bertini cascade inelastic scattering was desirable due to it's accuracy at these energies[9]. The physics list QGSP_BERT and QGSP_BERT_HP ('BERT' specifying Bertini cascade) were thus chosen as they both utilize Bertini cascade. The HP list is used whenever neutrons are generated since QGSP_BERT fails to accurately transport low energy (less than 20 MeV) neutrons and QGSP_BERT_HP utilizes more detailed neutron cross sections whenever possible and otherwise uses the Low Energy Parameterized model for these neutrons.

B. Volumes

The other main part of a simulation in Geant4, volumes, works via a hierarchy: there is one *world volume* describing the extent of the simulation and many trees of nested volumes within the world. No object can be outside of the world and particles are deleted as soon as they exit the world. The nested volumes are called *physical volumes* and act as complete descriptions of the object. These volumes are based off *logical volumes*, simpler descriptions without position or rotation. Logical volumes are, in turn, based off *solid volumes* which only specify size/shape.

These volumes may either be specified directly in the C++ code or in an external file that Geant4 loads. The most natural file format for Geant4 and the one used in this paper is GDML (**G**eometry **D**escription **M**arkup **L**anguage). GDML files specify volumes in much the same way as in C++ except is done in XML, a widely used markup language.

C. Scoring

To record and output data from simulations, a process called 'scoring', must be implemented, specifying what should be measured and where. One method to score is to set a volume as a detector so whenever the specific quantity is deposited/flows through it, the data is recorded. This is useful for complicated detector geometry but volumes cannot be subdivided and thus this method is not useful for radiation simulations where grids of quantities are desired.

A second method (the one primarily utilized in this paper) is *command line scoring*. This separates the geometry from scoring by first building the world and then, after everything is built, specifying where and what should be measured. The scoring object is then called a *mesh/scoring grid* and can be placed anywhere and easily be subdivided. This is a benefit over the first method because, to measure a value in a rectangular grid in the first method, for example, one would need to generate a volume for each box in the grid even if some/all of those volumes are not physical. Furthermore, this method can be used to measure quantities in locations that the first method cannot since Geant4 treats the scoring grid slightly differently than a grid of volumes, so normal restrictions on where a volume can be placed are lifted.

D. Running a Simulation

Once the world has been developed, a particle is given all the properties needed to define its state (mass, position, charge, momentum, etc.). Afterwards, the Geant4 framework handles propagation of particle through matter, ending only when the particle exits the world volume or has too little energy. If one of the physical processes were to generate a secondary particle, then it is generated in a parallel simulation and Geant4 follows that particle in the same way that it followed the primary. It should be noted that Geant4 does not allow for space charge simulations: particles do not interact with each other.

IV. DOSING FUNCTIONS

A. Equivalent Dose

A common and well trusted measure of radiation damage is *equivalent dose*. Instead of measuring energy absorbed per unit mass, as dose deposit does, equivalent dose applies an extra weighting function based on the particle type and energy. The traditional units of equivalent dose are rem (**R**oentgen **e**quivalent **m**an) with 1 rem increasing ones lifetime cancer likelihood by 0.005%[10]. This definition illuminates how weighting factors are determined: the amount of dose, C, required to increase cancer likelihood by 0.005% is found and then the weighting factor for that particle and energy is $W = 1/C$, where the dose is in units of rad.

At Cornell, the yearly equivalent dose limit for non-radiation workers is 100 mrem, matching the value put forward by the United States Nuclear Regulatory Committee (NRC 10 CFR 20.1201). Thus, the largest permissible increase in lifetime cancer likelihood over 1 year is 0.0005%.

B. Flux Method

The weighting method fails to accurately calculate ambient equivalent dose due to the inherent assumption that the dose deposited is in water. Another method of calculating equivalent dose, used in ICRP 21[11], instead weights the particle flux, not dose deposit, to get equivalent dose. This method both circumvents the issues with calculations of ambient quantities and MCNP uses it, so it is chosen for the Geant4 scorer. The weights for the gamma and neutron flux are shown in figures 1 and 2, respectively.

To calculate equivalent dose given a beam of electrons hitting a target in this way, the Geant4 scorer needs *cell flux* per electron (another measure of particle flux), F, primary rate, e^-_{rate}, the radiation types, R, and radiation energy, E. The equivalent dose rate, H_{rate}, then is calculated via equation 1:

$$\frac{H_{rate}}{\mathrm{mrem/h}} = \sum_R W_R(E)^{-1} \cdot \frac{F}{R\,\mathrm{cm}^{-2}} \cdot \frac{e^-_{rate}}{\mathrm{s}^{-1}} \tag{1}$$

where $W_R(E)$ is the weighting function depending on radiation type and energy.

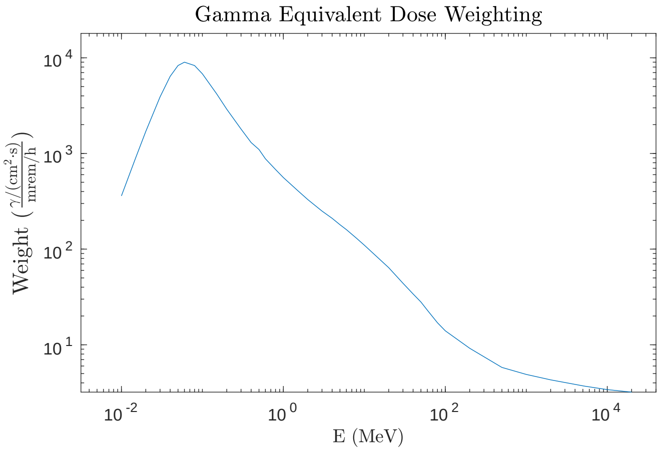

FIG. 1. Weights for conversion of gamma flux to equivalent dose published by ICRP 21.

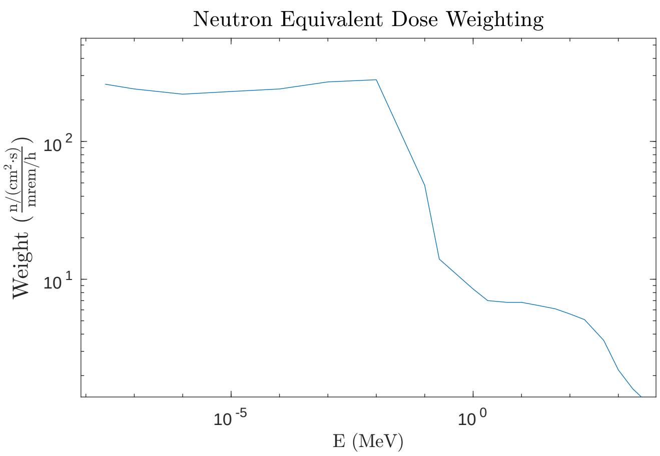

FIG. 2. Weights for conversion of neutron flux to equivalent dose published by ICRP 21.

V. BENCHMARKING

A. Scorer Test

To validate the scorer, a benchmarking experiment of shooting 5 million 50 MeV electrons into a 1 inch radius and 0.5 inch thick aluminum slug was performed. This slug was placed at the center of the world and a 98 x 98 x 2cm lead screen was placed at (0, 0, 48.5)cm to catch the showering particles. The setup is detailed in table I and displayed in figure 3.

Object	Material	Size	Location (cm)
Particle Source	N/A	N/A	(0, 0, -20)
Slug	Aluminum	$r = 1$", $t = 0.5$"	(0, 0, 0)
Screen	Lead	98 x 98 x 2 cm	(0, 0, 48.5)

TABLE I. Table of geometry setup parameters for the equivalent dose benchmarking test. Note that r stands for radius and t stands for thickness.

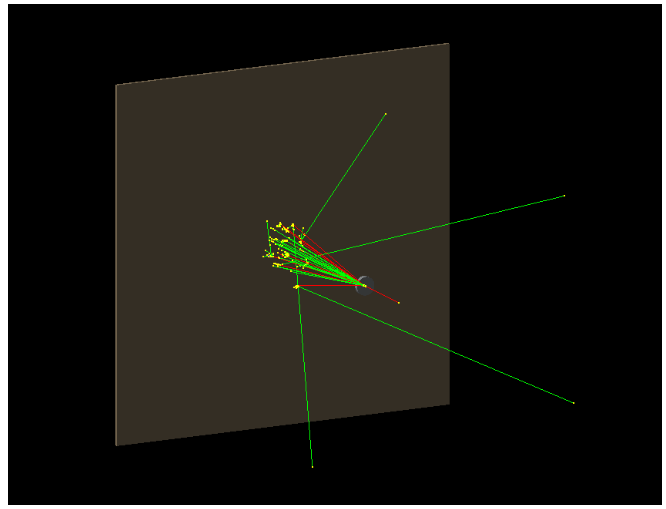

FIG. 3. Photo of equivalent dose benchmarking test with 10 electrons shot in Geant4.

This simulation was performed both in Geant4 and MCNP and, as shown in figure 4, the gamma cell flux and equivalent dose match extremely well at most locations, only diverging at the peak by a factor of approximately 1.24 and 1.38 for cell flux and equivalent dose, respectively. As the equivalent dose is based off the cell flux, the existence of such a similar discrepancy indicates the cause of the difference is not in the equivalent dose scorer, but most likely in a fundamental difference in how Geant4 and MCNP track particles. Nonetheless, the error is not large and thus not overly concerning.

There is more significant discrepancy when comparing the neutron cell flux and dose from Geant4 and MCNP. As shown in figure 5, the neutron cell flux differs, indicating an error in fundamental simulation method. The resultant discrepancy in the equivalent dose mostly matches that in cell flux discrepancy but is markedly worse (factor of approximately 1.56 and 2.34 for cell flux and equivalent dose, respectively, at the peak). This indicates that the error is likely mixed between the neutron flux and the equivalent dose scorer. In any case, the difference between neutrons is relatively modest (same order of magnitude) and thus not debilitating.

B. Material Test

This framework was primarily developed for radiation shielding simulations of the CBETA particle accelerator. As CBETA commonly uses concrete and high density concrete for shielding[12] (table III in the appendix for material definitions), these materials are benchmarked to ensure accuracy. To perform this test, 6 MeV photons, neutrons, and electrons were shot at a 2 x 2 x 2m box of plain and reinforced concrete, and both cell flux and equivalent dose were scored. As expected, the particle beam exponentially decays as it pierces through the ma-

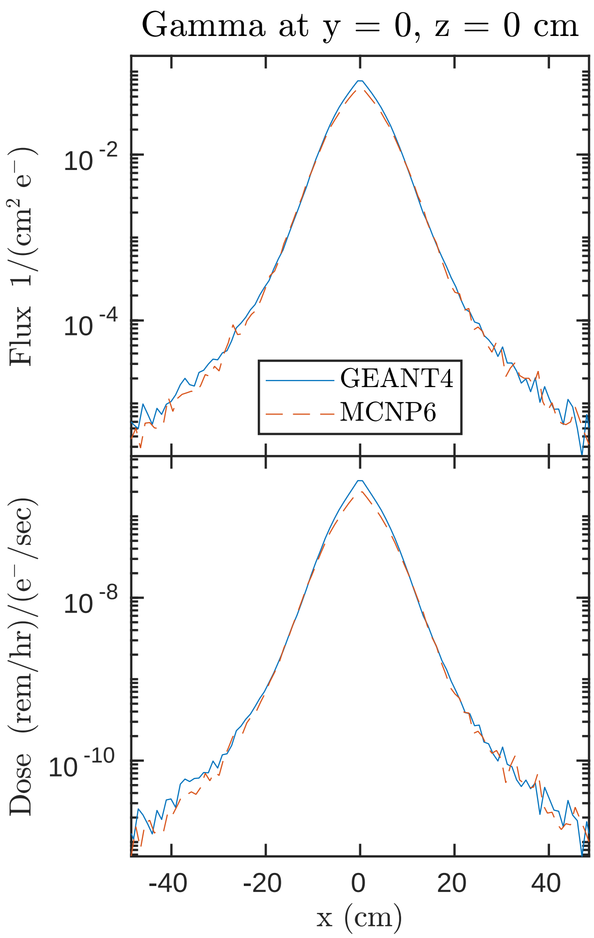

FIG. 4. Comparison of flux and equivalent dose for gamma radiation in the equivalent dose benchmarking test at the center of the lead screen (local coordinates (x, 0, 0)cm). The solid blue line represents Geant4 and the dashed red line represents MCNP. The data matches very well except for a discrepancy of approximately 1.24 and 1.38 for cell flux and equivalent dose, respectively, at the peak.

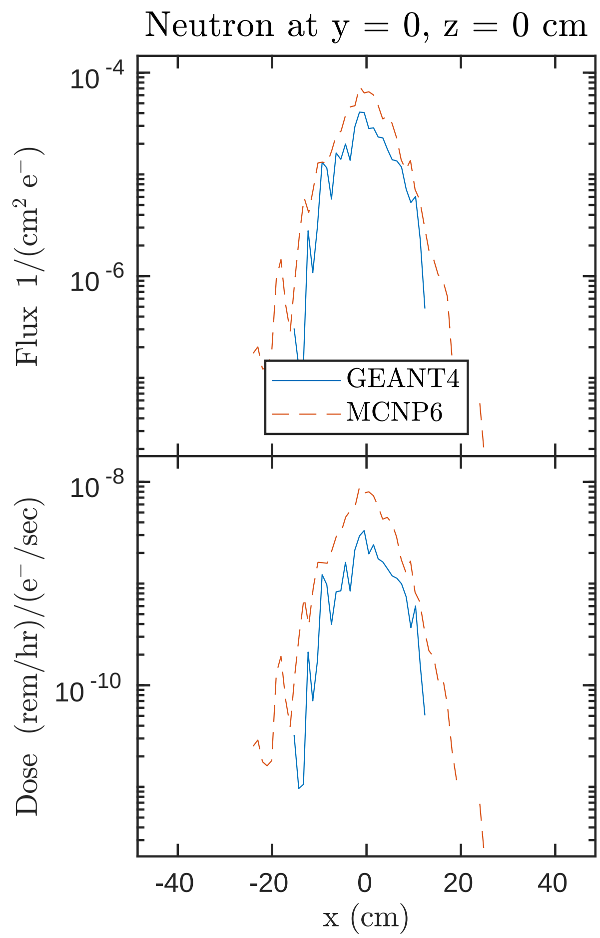

FIG. 5. Comparison of flux and equivalent dose for neutron radiation in the equivalent dose benchmarking test at the center of the lead screen (local coordinates (x, 0, 0)cm). The solid blue line represents Geant4 and the dashed red line represents MCNP. The data is of the same order of magnitude (discrepancy of factors of approximately 1.56 and 2.34 for the cell flux and equivalent dose at the peak, respectively) but there is more discrepancy than gamma radiation.

terial box in in the Geant4 simulations (see figures 9 and 10 in the appendix). The same simulation is being performed currently in MCNP and while there are no results yet, low particle count tests show similarity.

VI. GEOMETRY INTERFACE

While the CBETA accelerator has already been modeled in Autodesk inventor, Geant4 cannot naturally import it as it does not parse any exportable 3D model from Solidworks or Autodesk inventor. It would be tedious, time consuming, and error prone to remake the whole accelerator by hand in any new format. Therefore a geometry conversion method is desired to transform CAD files to GDML. This is not a desire unique to CBETA so, with the goal of a general framework, this interface should be as flexible as possible.

In order to convert an Autodesk Inventor model to GDML, the CADMesh package[13] was implemented. This package allows importation of STL files to Geant4, and the GDML parser built into Geant4 may then be used to export the geometries to GDML. STL files are common and easily exportable, making this framework generally usable. Further, as this method can theoretically accept any STL file, it is powerful enough for current simulations. For example, see figure 6, the S1.PIPE.01 beam pipe converted to GDML.

As Geant4 imports STL models as single volumes, only one material can be applied to them. To model many materials, the STL files are broken into logical pieces such as the shielding walls and beam pipes. This has the benefit of allowing easy enabling/disabling of volumes via modifying the mother GDML file, a file that links together all subsections. Another upside of this method is that the geometry is segregated from the simulation framework,

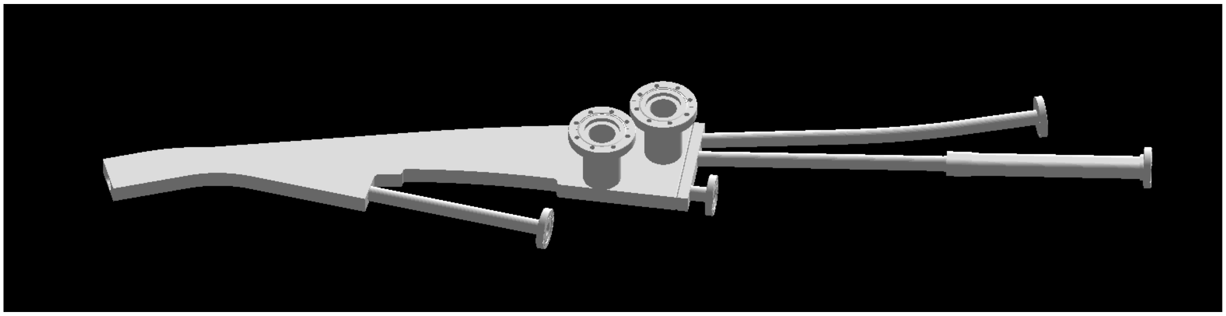

FIG. 6. S1.PIPE.01 beam pipe imported to Geant4 via CADMesh

allowing the framework to more easily be used for many simulations.

As the STL file format is a tessellated geometry, so are the GDML files. This has the downside of GDML files created in this manner not being very readable compared to human-made GDML files that can utilize Geant4 geometries like cylinders, boxes, and spheres. However, this downside would occur for any geometry conversion method.

VII. CBETA SIMULATIONS

This software was developed for the purpose of simulating radiation patterns in single point full beam loss scenarios for the CBETA particle accelerator. This occurs when a dipole steering magnet fails and electrons collide with the beam pipe wall. To ensure safety, the dose rate should not exceed approximately 0.0114 mrem/h, the value that a person can receive continuously for a year and still stay under the NRC dose limit.

There are many failure locations which are being tested but currently only seven have been analyzed, as shown in table II. These simulations use the FAT shielding configuration as it is what will be run first, so there is an urgency to ensure it is safe. The two primary areas of concern are the public zone (roughly from z=0.6m to z=19.2m and x=-0.9m to x=5.8m) and the equipment zone (upper right corner). The equipment zone contains many sensitive pieces of equipment which, while more resilient than human beings to equivalent dose, are still sensitive[14, 15].

An example simulation run with 100 million 42 MeV electrons hitting S1.PIPE.01 and being transported by QGSP_BERT_HP is shown in figures 7 and 8. In these simulations, the equivalent dose was analyzed via taking the maximum dose value from a 2D convolution, averaging over 30 x 30 pixels in a box at beam height from z=0.6m to z=19.2m and x=-0.9m to x=5.8m. This box was chosen as it roughly encompasses the public zone. The results from these simulations are listed in table II with all simulations showing comparable dose rates to MCNP simulations. These rates are slightly higher than were measured, but that is to be expected as the simulations exclude many objects around the beam pipe that likely absorb significant radiation such as the dipole and quadrapole magnets. Even a simplified model of the magnets may significantly reduce discrepancy.

Location	Energy (MeV)	Max Gamma Dose Rate (mrem/h)	Max Neutron Dose Rate (mrem/h)
A3.SWYD	6	8.373	0
B1.PIPE.01	6	18.515	0
B1.PIPE.02	6	26.927	0
S1.PIPE.01	42	56.738	12.967
S1.PIPE.02	42	29.528	7.676
S1.PIPE.03	42	30.420	9.407
S1.PIPE.04	42	30.803	13.394

TABLE II. CBETA failure locations and public dose results from simulations with 100 million particles for all locations except for S1.PIPE.02, which was run with 40 million for now.

VIII. CONCLUSION

In sum, a radiation shielding simulation framework was developed in Geant4, allowing for streamlined geometry generation and accelerator failure simulations. The framework accepts the commonly used 3D model format STL (via CADMesh), and converts it into GDML, an efficient and flexible format for such simulations. Custom scorers have been generated utilizing the equivalent dose calculation method described in ICRP 21[11] and have been tested against MCNP's equivalent dose scorers, showing good agreement. Additionally, a benchmarking test for the plain and heavy concrete used in CBETA shielding was performed with Geant4 showing exponential decay as expected; the MCNP simulations are in progress. Lastly, shielding simulations were performed for seven locations in the CBETA particle accelerator and more are being performed as this paper is written.

More benchmarking between Geant4 and MCNP is called for to verify that they give the same results and, if not, to give clues as to the source of the discrepancy. Furthermore, the discrepancy between simulation and experiment must be investigated beginning with the addition

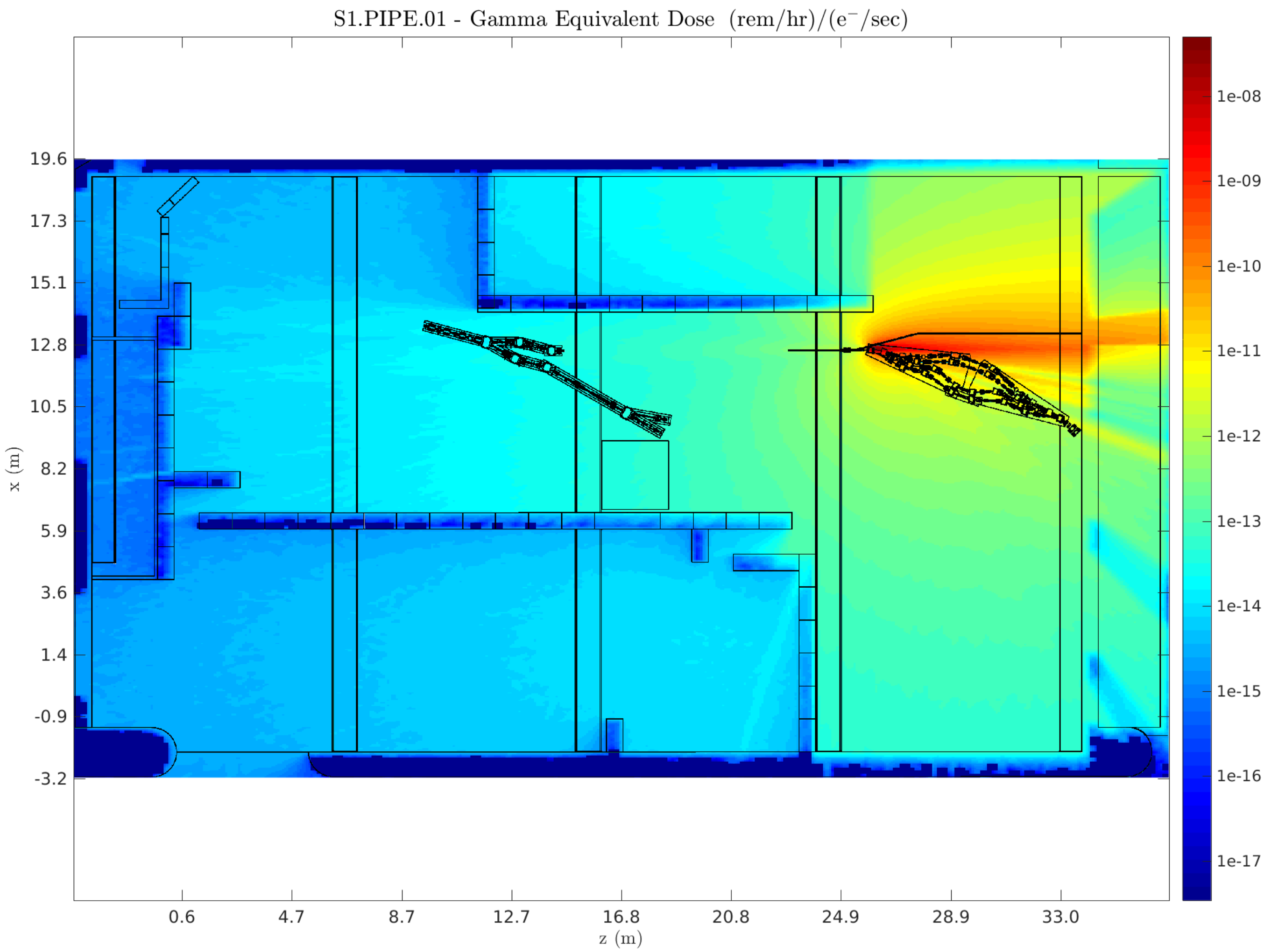

FIG. 7. Logarthmic colormap of gamma dose in the S1.PIPE.01 single point full beam loss scenario.

of similar objects. Lastly, new scoring methods such as effective dose should be generated and evaluated. When this is built, standard human phantoms can be generated and used not only to validate the scorers, as ICRP has tabulated data for dose rates on such phantoms, but also to obtain more information on the radiation danger of magnet failure on a human phantom.

IX. ACKNOWLEDGMENTS

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X. APPENDIX

A. Material Tests

A collection of concrete shielding data is collected, including the isotopic composition of the concrete and the exponential decay of radiation through it.

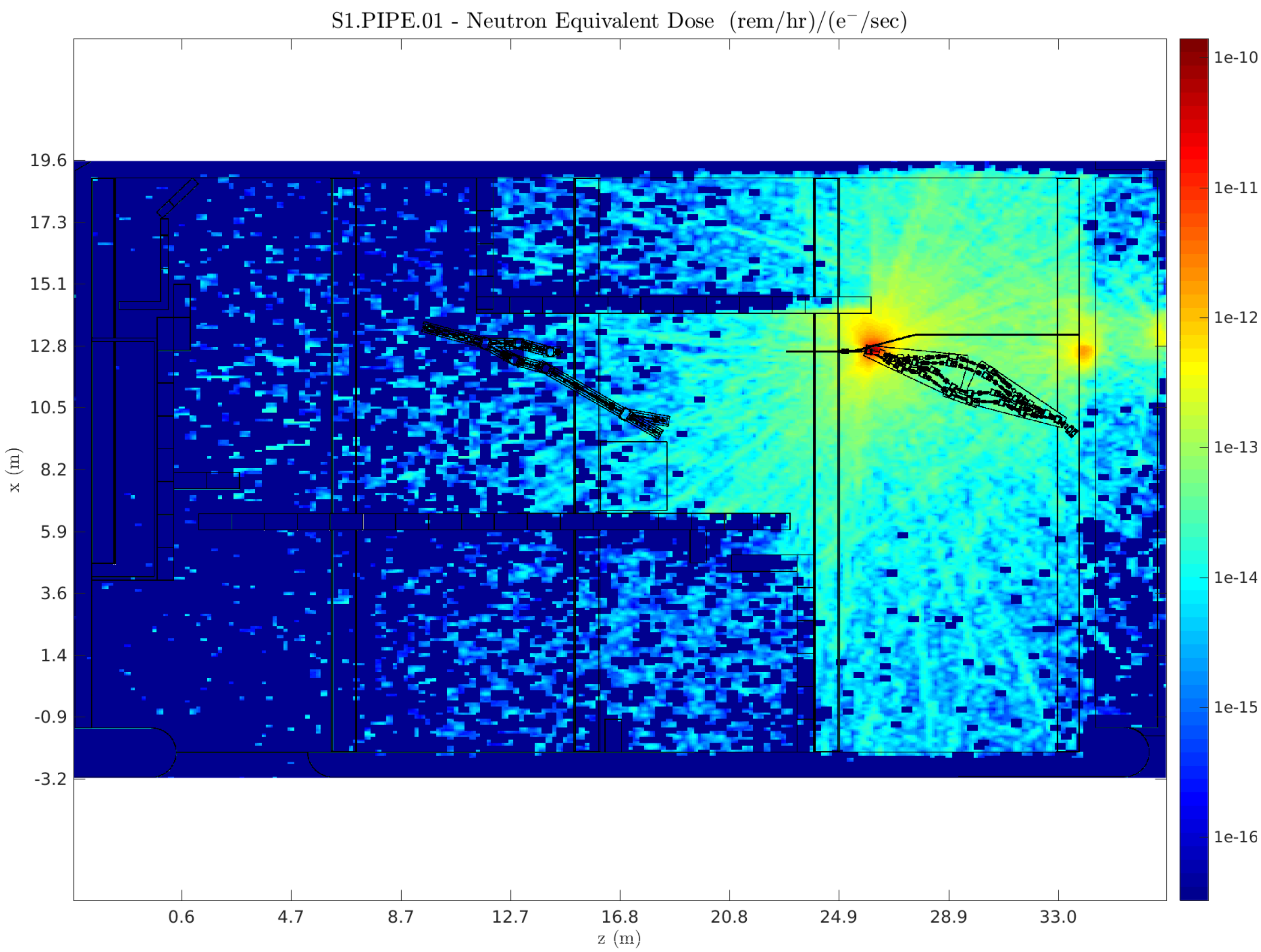

FIG. 8. Logarthmic colormap of neutron dose in the S1.PIPE.01 single point full beam loss scenario.

Isotope	Plain Concrete	Reinforced Concrete
$^{1}_{1}H$	0.5558%	0.3760%
$^{16}_{8}O$	49.6746%	30.439%
$^{17}_{8}O$	0.0204%	0.013%
$^{18}_{8}O$	0.1126%	0.069%
$^{23}_{11}Na$	1.7101%	0.011%
$^{24}_{12}Mg$	0.1999%	0.124%
$^{25}_{12}Mg$	0.0264%	0.016%
$^{26}_{12}Mg$	0.0392%	0.019%
$^{27}_{13}Al$	4.5746%	0.320%
$^{28}_{14}Si$	28.9488%	0.957%
$^{29}_{14}Si$	1.5181%	0.050%
$^{30}_{14}Si$	1.0423%	0.034%
$^{31}_{15}P$	0%	0.004%
$^{32}_{16}S$	0.1216%	0.072%
$^{33}_{16}S$	0.0010%	0%
$^{34}_{16}S$	0.0057%	0%
$^{39}_{19}K$	1.7882%	0.051%
$^{41}_{19}K$	0.1357%	0%
$^{40}_{20}Ca$	8.0175%	3.934%
$^{42}_{20}Ca$	0.0562%	0%
$^{43}_{20}Ca$	0.0120%	0%
$^{44}_{20}Ca$	0.1898%	0%
$^{48}_{20}Ca$	0.0186%	0%
$^{48}_{22}Ti$	0%	0.012%
$^{54}_{26}Fe$	0.0707%	3.588%
$^{56}_{26}Fe$	1.1390%	58.352%
$^{57}_{26}Fe$	0.0265%	1.372%
$^{58}_{26}Fe$	0%	0.184%

TABLE III. Isotope definition of Plain Concrete and Reinforced Concrete used for CBETA shielding.

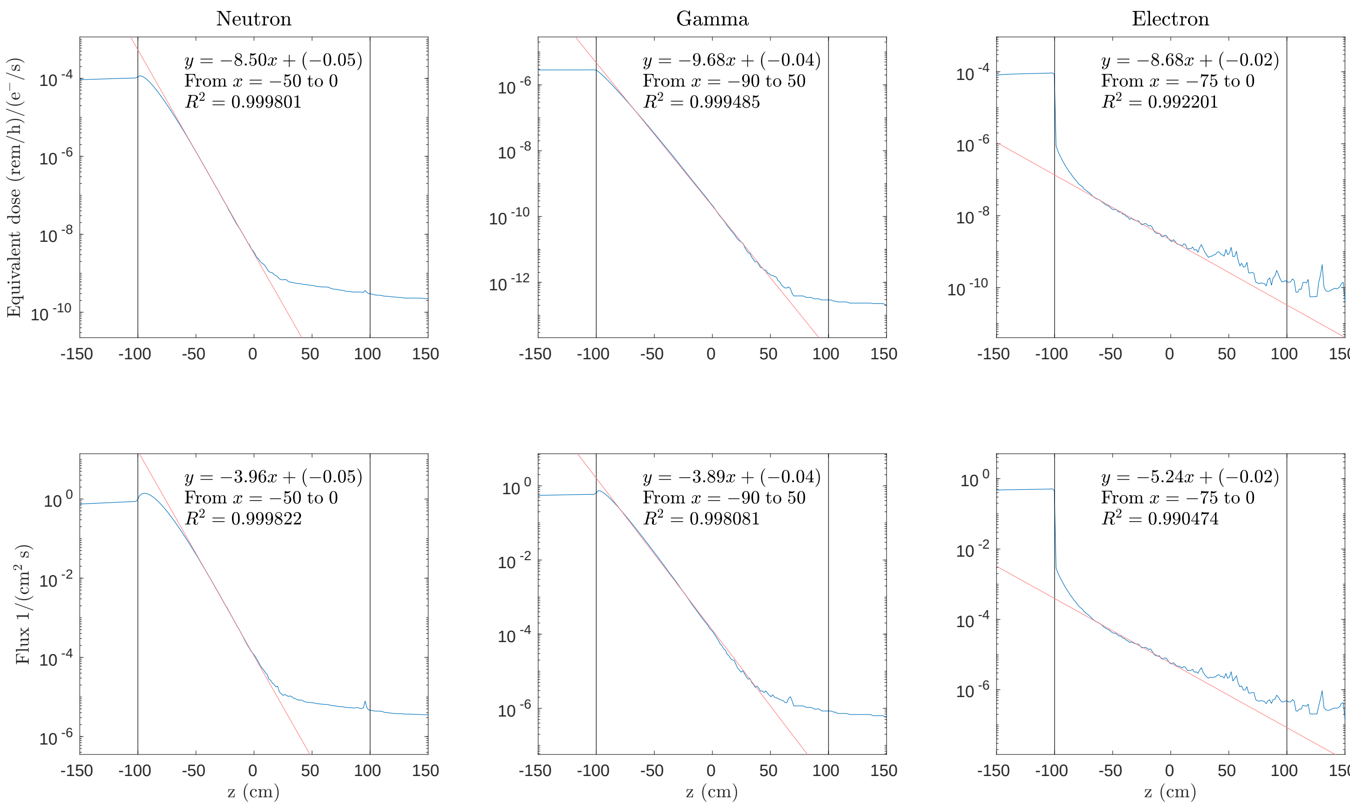

FIG. 9. Benchmarking test for 6 MeV neutrons, photons, and electrons shot into a 2 x 2 x 2m reinforced concrete box (zone in between the black lines). Given the beam shot in the z-direction, the plots are the measured quantities integrated over x and y. All plots show exponential decay, as expected.

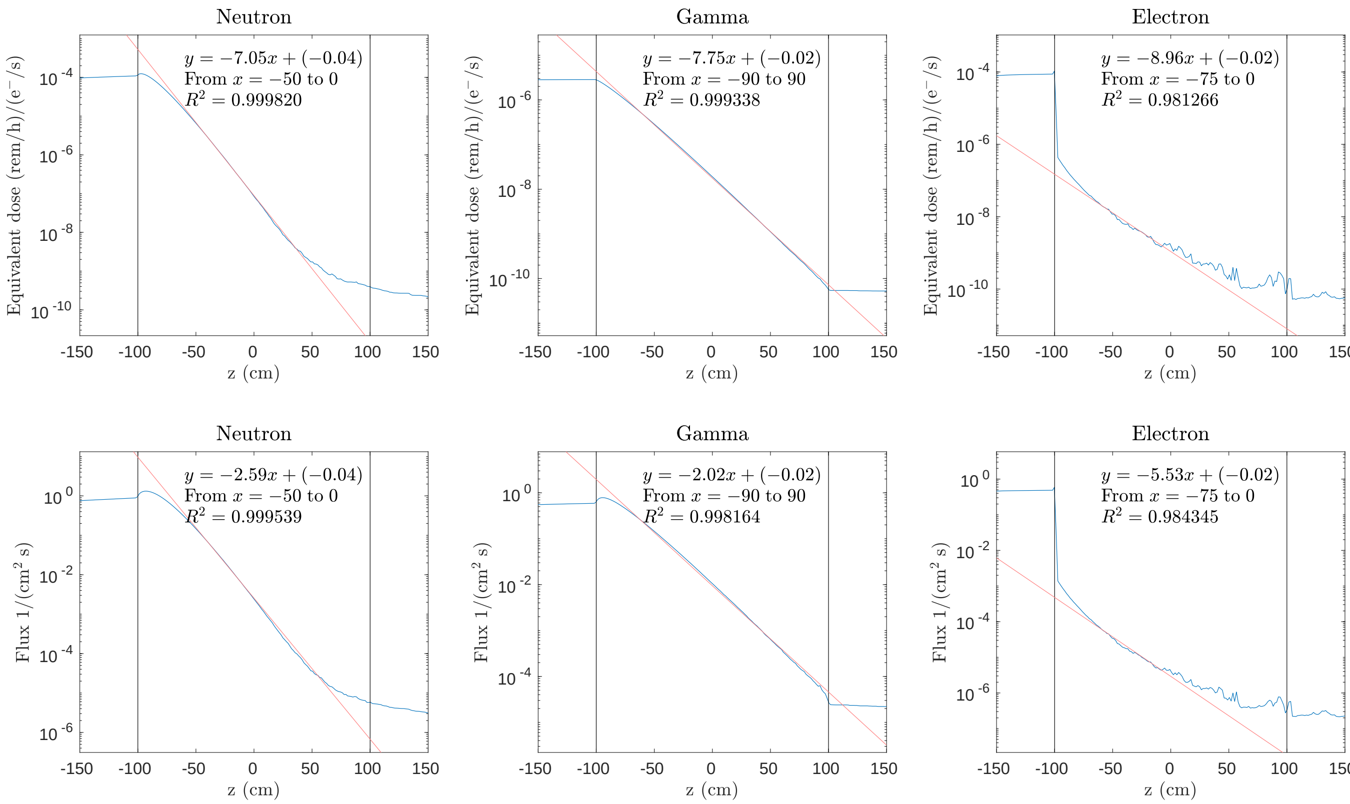

FIG. 10. Benchmarking test for 6 MeV neutrons, photons, and electrons shot into a 2 x 2 x 2m plain concrete box (zone in between the black lines). Given the beam shot in the z-direction, the plots are the measured quantities integrated over x and y. All plots show exponential decay, as expected.

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