Modeling low energy x-ray interactions with biological material at the CUEBIT

Journal of Physics: Conference Series **583** (2015) 012046 doi:10.1088/1742-6596/583/1/012046

Modeling low energy x-ray interactions with biological material at the CUEBIT

J Klingenberger[1], M Schott[2], T Kimmel[3], D Medlin[3], A Gall[3], M Rusin[4], D Dean[4], E Takacs[3]

[1]School of Computing, Clemson University, 100 McAdams Hall, Clemson, SC 29634, USA
[2]Department of Electrical Engineering and Computer Science, Vanderbilt University, 400 24th Ave S Jacobs Hall, Nashville, TN 37212, USA
[3]Department of Physics and Astronomy, Clemson University, 118 Kinard Laboratory, Clemson, SC 29634, USA
[4]Department of Bioengineering, Clemson University, 301 Rhodes Research Center, Clemson, SC 29634, USA

E-mail: klinge2@clemson.edu

Abstract. Recent developments at Clemson University have established the need to model the production of x-rays using a highly charged ion beam generated by the Clemson University Electron Beam Ion Trap (CUEBIT). A Geant4 modeling environment has been developed on Clemson University's Palmetto2 supercomputing cluster to simulate the interaction of these x-rays with biological material. Preliminary results of the model have been obtained after performing initial simulations on the computing cluster. Future experiments using the CUEBIT as well as refinements to the Geant4 model are discussed.

1. Introduction

Understanding the primary and secondary effects of radiation on biological material is difficult given the small distance and time scales of these interactions. The primary interaction is either a photoionization or a photon scattering effect that takes place somewhere along the path of the incoming x-ray. The secondary processes include electron scattering events leading to a cascade of chemical and biological events. At Clemson University's Electron Beam Ion Trap (CUEBIT), experiments are being performed involving the irradiation of biological material with low energy x-rays. Monte Carlo computer simulations of x-rays interacting with biological material are also being constructed in an effort to better understand the multi-step processes that lead to measurable effects on the cell function. Importantly, the simulations need to be accurate so that any conclusions made are correct and verifiable. A main goal of the CUEBIT simulations is to track secondary interactions inside biological material that occur as a result of chemical or biological processes.

The computer simulations that model x-rays output by the CUEBIT can be verified by performing experiments with the physical machine. Verification can be done by recording the amount of dose deposited by a phantom in the simulated experiment and comparing the results to a phantom placed in an irradiation chamber attached at the end of the real, physical CUEBIT machine.

Recent publications suggest that low energy radiation may cause a cascade of effects on biological material [1]. A main goal of the CUEBIT simulations is to track these secondary interactions inside biological material that occur as a result of biological or chemical processes. Modeling the pathways of these processes using Monte Carlo simulation software will provide further understanding of these effects.

Using computers to perform Monte Carlo simulations of physical processes is not new. The high-energy physics group CERN maintains a freely obtainable particle simulation toolkit called Geant4 [2]. This software provides a programming environment to instantiate particles with arbitrary properties and run a simulation with user-defined particle interactions enabled. While Geant4 was developed in the scope of high-energy physics, the program is now general purpose enough that simulations of low energy interactions are also possible. Additionally, a medical physics simulation package called GATE [3] has been built on top of Geant4, which provides useful features to simplify common tasks in radiation therapy simulations. GATE is an appropriate program for simulating experiments at the CUEBIT due to its Geant4 base and its additional functionality such as dynamic simulations over time.

In this paper, methods for collecting data from GATE simulations will be described. Additionally, simplifications made in regard to this preliminary modeling work will be explained, as well as refinements to be made in the future. Lastly, a technique for speeding up the runtime of simulations through the use of a supercomputing cluster will be detailed.

2. Results and Discussion

Initial results from a GATE simulation of a model of an irradiation port at the end of the CUEBIT have been generated. In this section, the construction of the model and methods for manipulating the model to extract useful data are discussed. The simulation that was developed is a model of a physical experiment that is planned for the CUEBIT. A hollow irradiation chamber at the end of the highly charged ion beam line curves the beam using a quadrupole bender so that the ion beam is directed vertically upward. At the top of the irradiation chamber, a beryllium window is placed so that the ions impact the window. Upon impact, charge exchange occurs between the highly charged ions and the beryllium window, causing a cascade of interactions that ultimately release low energy x-rays. On top of the irradiation chamber, a cell flask is placed on an irradiation port in the path of these x-rays.

2.1. Description of the model geometry

In order to provide useful data, the model used by the simulation needed to be accurate. Particularly, the thickness of certain materials affects the penetration depth of x-rays. Special consideration went into the choice of material for the bottom of the cell flask, since most common flask materials such as silicate glass absorb x-rays in the energies emitted by the beryllium window. In this design, a cell flask bottomed with a thin Mylar membrane is employed, since Mylar is transparent to x-rays in the energy region of interest [4]. Therefore, it is important to include the layer of Mylar between the x-ray source and cell medium in the model with accurate dimensions.

Biological materials are complex subjects to model. While future refinements of the biological material used in the model are planned, the current model approximates the biological material with a volume of pure water. Given that biological material is largely composed of water, the x-ray dose applied to water should not be significantly different than a dose of x-rays applied to biological material.

2.2. Input of the x-ray energy distribution

Particle simulations are computationally intensive programs. Therefore, it is useful to isolate and track interactions in parts of the system that have a direct effect on the experiment of interest. The distribution of x-ray energies generated through charge exchange processes on the beryllium window can be measured using an x-ray spectrometer. The experimental values obtained from this spectrometer can then be input into the model using a command built into GATE. X-rays are then

generated according to this distribution at the x-ray source in the model, which makes the model physically accurate.

However, the x-ray energy distribution generated by the beryllium window at the CUEBIT has not yet been obtained. In absence of this distribution, x-ray energies of exactly 3.0 keV and 3.5 keV from the known ion decay process were used. These values were approximations of the expected values to be generated by the CUEBIT in this initial modeling work. The choice to use an x-ray distribution rather than model the ion decay and decay product generation was intentional. An x-ray energy distribution collected through experiment will be used as input as soon as such data is available.

2.3. Collection of the absorbed dose data

A computer simulation of an experiment would have no purpose in a scientific context if data could not be extracted from the simulation. GATE offers a useful feature called "actors" that allow for functions to be executed at different stages of the simulation. One particular actor that is useful is the DoseActor. With the DoseActor enabled, the energy deposition into a given volume can be output into a file in a voxelized format such as ROOT or MetaImage. In the simulation model of the CUEBIT experiment (Figure 1), the DoseActor is particularly useful since the deposition of energy can be collected on a per volume basis. A more refined model with volumes representing individual cells will enable energy deposition to be collected per cell basis.

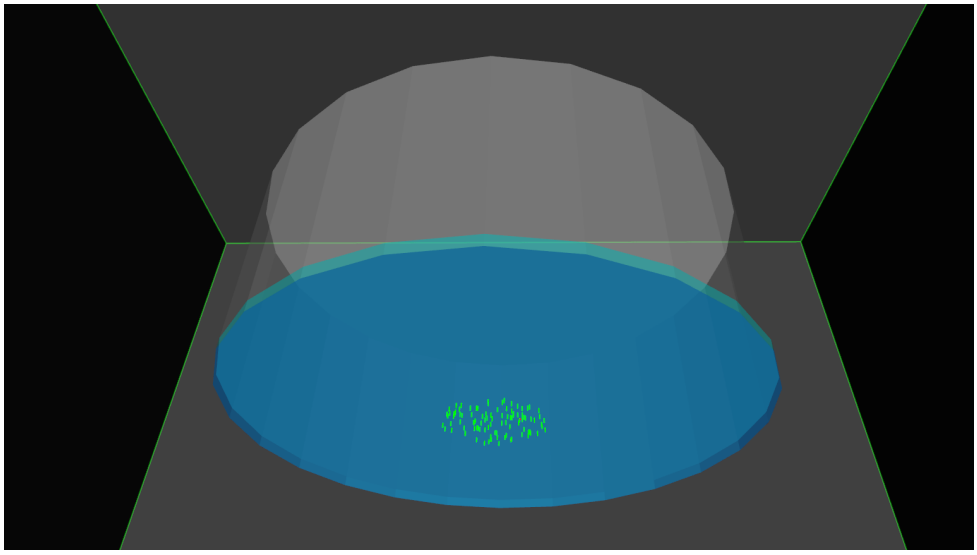

Figure 1. Visualization of the flask irradiation. The gray cylinder is the cell flask, which is filled with a water substrate (bottom of flask). Generated x-rays strike the flask from below.

2.4. Parallelization of the simulation

The complexity of a simulation increases as the number of particles to track increases and as the number of volumes increases, and subsequently the amount of time a simulation takes to complete also increases. Therefore, it is often desirable to simplify a simulation where possible. A parallelization technique was used on the model of the CUEBIT irradiation chamber that enabled multiple particles to be tracked simultaneously. By running the same simulation in multiple processes on the Palmetto2 supercomputing cluster, statistics on energy deposition into the biological material volume could be generated in less time. The speed improvement increases approximately linearly as the number of threads performing the simulation increases. While the current experimental model is not of sufficient complexity to warrant such optimizations, future refinements of the model will contain several thousand volumes of individual cells. Using a supercomputing cluster will provide the critical

performance boost needed to compute the simulation with enough particles to guarantee adequate statistical results in a reasonable timeframe.

3. Conclusion

Constructing computer simulations of experiments at the end of the CUEBIT has been shown to be useful in predicting where the majority of the interactions of x-rays with biological material take place. The data collected from models can be compared to results from the irradiation chamber to verify that the models reflect reality. While the current model of the irradiated cell flask contains only a water substitute for biological material, this model will be refined to have cell volumes that contain subvolumes that model organelles. Current Monte Carlo particle tracking packages only model physical interactions, so more work is required to model the chemical and biological effects relevant to the biological material being studied. With the appropriate interactions simulated and a high detail model of the biological material including cellular components, more details of the primary and secondary effects that lead to cell death may be better understood. However, such simulations are computationally expensive on current mid-range hardware, so efficiency optimizations such as parallelization of the simulation are critical to performing the simulations in a reasonable amount of time.

Acknowledgements

NASA EPSCoR Palmetto Academy Program
Clemson University Creative Inquiry (CI) Program
Clemson University Professional Internship & Co-Op (UPIC) Program
Clemson University REU Program in Data-Intensive Computing
Department of Physics and Astronomy at Clemson University

References

Giedzinski E 2013 *Rad. Res.* **164** 540
Allison J *et al* 2006 *IEEE Trans. Nuc. Sci.* **53** 270
Jan S *et al* 2004 *Phys. Med. Biol.* **49** 4543
Medlin D, Heffron W, Siegel A, Wilson R K, Klingenberger A, Gall A, Rusin M, Dean D, Takacs E 2014 *J. Phys.: Conf. Series* (Submitted)