CMPE 491 - ODYSSEUS (Optimized Deep-learning for Shielding Systems and Energy Usage Simulation)

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June 7, 2023

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1. INTRODUCTION

1.1. Broad Impact

In the context of wearable protective materials, our project aims to use deep learning techniques to build an Artificial Neural Network (ANN) model that can predict the outputs produced by the PENELOPE Monte Carlo simulator for specific materials and geometries. The objective is to drastically cut down the time needed for material design tasks while maintaining PENELOPE simulations' degree of precision and dependability. We intend to prepare a scientific article to share our findings and contribute to the scientific literature.

1.2. Ethical Considerations

The development and implementation of ODYSSEUS for material design should take into account any potential ethical issues, as with any new technology. Key ethical issues that need to be addressed include the following:

Decisions made by the AI tool will have an impact on the actual world, even in the medical area. Ensuring that the creators and users of the tool are responsible for any mistakes or unforeseen effects that may result from its use is important. Working with PENELOPE is crucial because the accountability of the simulation is very high.

The development of the AI tool involves the use of intellectual property owned by others, such as Penelope/PenEasy simulations or deep learning algorithms. We attach importance to ensuring appropriate citations and avoiding potential legal and ethical issues.

2. PROJECT DEFINITION AND PLANNING

2.1. Project Definition

PENELOPE is a Monte Carlo simulator for coupled electron-photon transport in arbitrary materials for a wide energy range. Photon, electron, and positron transport histories are generated considering the interactions according to material and geometry properties. For developing radiation-protecting materials, time-consuming simulations are carried out with different material combinations to optimize weight, cost, or some other metric while satisfying the requirements. Although PENELOPE is a high-precision and accurate Monte Carlo simulator, it is built on old technology and it cannot be parallelized.

In this project, we will be exploiting Artificial Neural Network (ANN) techniques -especially deep learning techniques- to eliminate the need for Monte Carlo simulations for selected materials and geometry that is in the scope of wearable protective materials. Hence, the required time for material design tasks will be improved significantly.

2.2. Project Planning

The creation of a project team, defining the project's scope, and identifying its stakeholders are the first steps in the process. Goals, objectives, and success criteria must be outlined, tasks and roles must be assigned, and a high-level project plan with deliverables and milestones must be developed.

The second phase entails researching Penelope/PenEasy simulation software to discover its advantages and disadvantages. Reviewing earlier research and scholarly writing, obtaining software access, specifying variables for wearable safety gear, and creating simulations to precisely reflect materials and geometries are all necessary steps in this process.

The third phase is developing simulations and collecting data in order to train and test the deep learning model. In order to prepare the simulation output data for use in the deep learning model, simulations must be created for a variety of system configurations and then run.

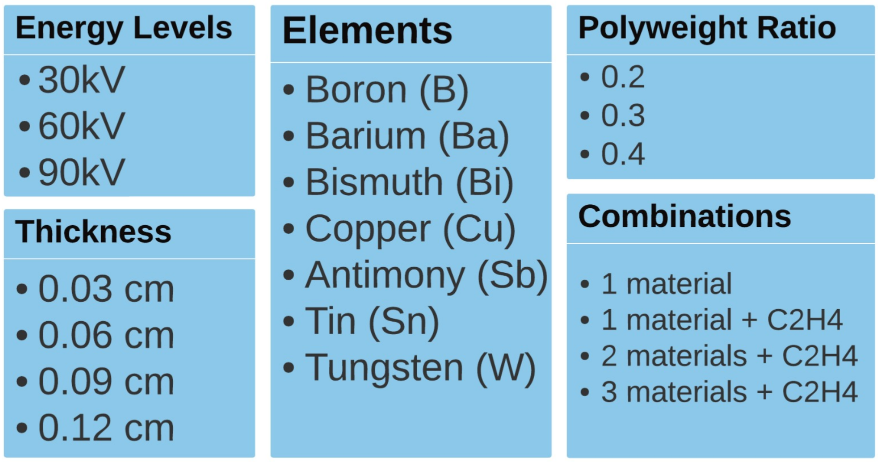


Figure 2.1. Simulation Plan

The creation of a deep learning model that can precisely anticipate simulation results is the fourth phase. This entails reading up on deep learning techniques, developing a precise model architecture, programming the model in the proper language and framework, and training and testing the model using the output data from the simulation.

Writing a scientific publication explaining the project's methodology, results, and conclusions is the fifth phase. This entails writing the essay in accordance with established standards, editing and revising it with input from stakeholders, and submitting the finished product to magazines or conferences that will publish it.

The project must be finished, its effectiveness evaluated, and any lessons learned noted as the last phase. This include conducting a project final analysis, documenting the project outcomes, and archiving relevant project materials.

2.2.1. Project Time and Resource Estimation

Penelope/PenEasy Simulation Investigation Phase

- Time: 2 weeks
- Resources: Penelope/PenEasy simulation software, literature resources

Simulation Data Collection Phase

- Time: 12 weeks (assuming we run 300 simulations per week)
- Resources: High-performance computing resources (CPU and GPU), Penelope/PenEasy simulation software

Deep Learning Model Design and Development Phase

- Time: 4 weeks
- Resources: Deep learning tools (Python libraries like Tensorflow, PyTorch), high-performance computing resources (CPU and GPU)

Scientific Paper Preparation Phase

- Time: 5 weeks
- Resources: Writing and editing tools (word processors, LaTeX), collaboration tools (Google Docs, Slack), relevant conferences or journals

Project Closure Phase

- Time: 1 weeks
- Resources: Project manager, communication tools

Total Time

- Total Time: 24 weeks

We will have the summer to work on this project, which will give us enough time to complete the project within the specified timeline and budget. In terms of computing resources, assuming each simulation takes between 4 and 4.5 hours, we estimate that we will need at least 3600 x 4 = 14,400 hours of CPU and GPU computing time. This will require access to a high-performance computing cluster or cloud computing resources. The exact resource requirements will depend on the specific computing environment and infrastructure available.

2.2.2. Success Criteria

The success of our project will be evaluated based on the following criteria:

(i) **Accuracy of the deep learning model:** When compared to Penelope simulations, the trained model should be able to predict the characteristics of new test materials with an accuracy of at least 96%. We will compare the actual values received from the Penelope simulations with the anticipated values generated by our model in order to evaluate the accuracy.

(ii) **Efficiency of the deep learning model:** Compared to Penelope simulations, the trained model should be able to produce predictions much faster. We will compare the time it takes to simulate a certain set of test materials using the Penelope software to the time it takes to produce predictions for that same set of test materials in order to determine how effective our model is.

(iii) **Generalization capability of the deep learning model:** The trained model ought to be able to adapt well to materials that aren't contained in the training data set. By assessing our model's performance on a set of test materials that are different from the training data set, we can determine whether or not it is capable of generalizing.

We will deem our project successful if our trained deep learning model can achieve these success criteria, with at least 96% accuracy and a vastly reduced calculation time compared to Penelope simulations.

2.2.3. Risk Analysis

(i) **Data Availability:** The depth learning model's performance may be impacted by the quantity and caliber of training data. Low data quality or limited data availability could put the performance of the model at risk. We will gather data from multiple sources and undertake data cleaning and preprocessing to assure the quality of the data in order to reduce this risk.

(ii) **Hardware Resources:** For the project to run simulations and train the deep learning model, extensive computer resources are needed. The possibility of having limited or inadequate hardware resources could result in project delays or subpar model performance. To reduce this risk, we'll make sure we have access to enough hardware resources, such the HPC clusters at our university, and we'll schedule the project properly.

(iii) **Model Complexity:** Deep learning models can be difficult to develop and apply, and there is a chance that doing so could result in overfitting or poor generalization. Alternately, the model could be overly straightforward and miss key aspects of the data. We will conduct a thorough literature analysis, speak with subject-matter specialists, and apply relevant methods, including regularization and cross-validation, to improve the model architecture in order to reduce this risk.

(iv) **Project Timeline:** The project timeline may be at risk due to unforeseen events, such as hardware failures, data collection delays, or unexpected project scope changes. We will carefully prepare the project schedule, work on it during the summer break, properly assign resources, and maintain communication among team members to reduce this risk. This will ensure that project milestones are completed on time.

(v) **Ethical and Legal Issues:** The usage of data or the trained model may raise ethical and legal concerns, such as data privacy or algorithmic bias. We shall carefully assess the ethical and legal ramifications of our activity, adhere to pertinent standards and laws, and seek the advice of subject-matter authorities as necessary to reduce this risk.

By identifying and mitigating these risks, we can increase the likelihood of project success and ensure that our work is carried out in a responsible and ethical manner.

2.2.4. Team Work (if applicable)

We, have broken the project down into distinct segments and intend to collaborate on each one. First, in order to better comprehend the software's advantages and disadvantages, we will both access the program and analyze earlier research on Penelope/PenEasy.

Second, we have chosen to divide the work of designing simulations and running them in order to gather data. To automate the simulations and gather the findings, we will each create unique script codes. Researching and analyzing various deep learning techniques, such as neural networks and other machine learning algorithms, for simulation estimates is our shared responsibility. To develop a deep learning model that precisely predicts the outcomes of simulations, we intend to work together and disseminate our discoveries. The paper will then be written and edited by both of us in accordance with customary standards for a scientific paper. To make the paper better, we'll also incorporate feedback from each other and other interested parties. To make sure the project stays on track and is successfully completed, we will work closely together and communicate often throughout.

3. RELATED WORK

While doing the literature review we mainly focused on two questions: Can ANNs learn material properties, microstructure, and compositions from data to predict their shielding properties accurately? Can the need for Monte Carlo simulations be eliminated by an AI tool that can predict the outcome of the simulation for specified inputs? In this section, we will document our findings of possible answers to these questions.

A few hundred eV to about 1 GeV in energy range, the computer code system PENELOPE (version 2014) conducts Monte Carlo simulation of coupled electron-photon transport in arbitrary materials. The typical, thorough simulation approach is used to model photon transit. On the basis of a combined technique that combines condensed modeling of soft interactions with a thorough simulation of hard events, electron and positron histories are constructed. Using a geometry program called Pengeom, homogeneous materials constrained by quadric surfaces, such as planes, spheres, and cylinders, may create random electron-photon showers. [1]

To save time and effort in setting up simulations, we use penEasy. It is simpler to set up and perform simulations with PenEasy [2], a graphical user interface for the PENELOPE Monte Carlo simulation tool. PenEasy's user-friendly interface makes it simple for researchers to quickly and simply build up simulations with the required input parameters, which simplifies the process of conducting simulations. A variety of tools are available on the interface for building intricate shapes, entering material information, and configuring simulation settings.

Deep learning techniques have been used for predicting the mechanical properties of materials based on their composition and microstructure. ANNs were used in a research by Lookman et al. to predict the mechanical characteristics of metals depending on their compositions. They showed the potential of ANNs for material design challenges by training their model on a huge dataset of material attributes and achieving

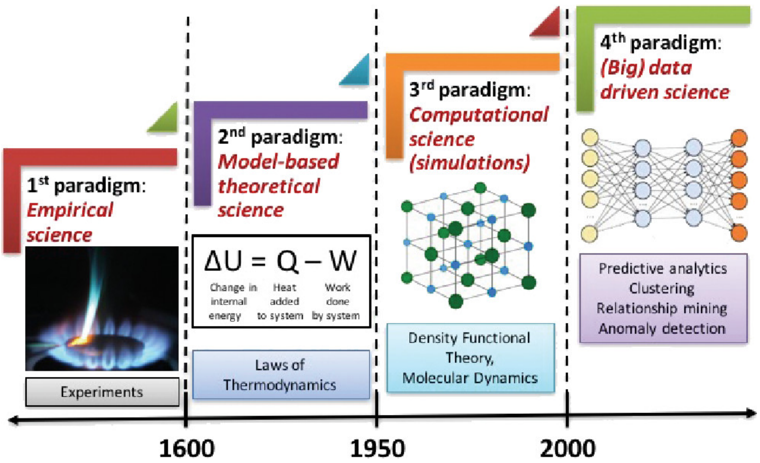


Figure 3.1. Four Paradigms of Science

high precision in their predictions. [3]

The use of artificial intelligence (AI) approaches to quicken Monte Carlo simulations in medical physics is suggested in the publication "Artificial Intelligence for Monte Carlo Simulation in Medical Physics" by A. Baroni et al. The authors talk about the difficulties with Monte Carlo simulations in medical physics, such as how expensive and time-consuming they are to run. They argue that AI methods like deep learning algorithms and artificial neural networks (ANNs) might be utilized to decrease the computing load and accelerate the simulations. The study offers a thorough assessment of the literature on the use of AI in Monte Carlo simulations, with illustrations of effective ANN and deep learning implementations in medical physics. [4]

4. METHODOLOGY

(i) Gathering simulation data from the Penelope/PenEasy simulator for various material and geometry settings is the initial stage in the project. A sizable dataset of simulation results for a variety of materials and geometries will be produced and gathered. To guarantee data quality and consistency, the collected data will be preprocessed and cleansed.

(ii) We will conduct exploratory data analysis to learn more about the properties of the simulation data, spot trends and connections between variables, and assess the accuracy of the information gathered. This will also assist us in selecting the proper engineering methods and feature selection strategies for the deep learning model.

(iii) We will develop and apply a deep learning model for estimating simulation outputs based on the exploratory data analysis. Regularization and cross-validation will be used appropriately to optimize the model architecture and prevent overfitting.

(iv) On a held-out test set of simulation data, we will assess the trained model's performance. Using relevant metrics, such as mean squared error or coefficient of determination, we will assess the model's predictions' accuracy. In order to assess how well the model stands up to changes in the input data, we will also do a sensitivity analysis.

(v) We will tweak and modify the model as needed to increase its accuracy and generalization performance based on the evaluation findings. This could entail adjusting the model's hyperparameters, using other feature sets or preprocessing methods, or using more data sources.

5. REQUIREMENTS SPECIFICATION

5.1. Glossary

- User: A person who runs the program.
- ODYSSEUS: Optimized Deep-learning for Shielding Systems and Energy Usage Simulation
- Material File: A '.mat'file generated by 'material.f' file in PENELOPE, that consists of information about the material's microstructure
- Configuration File: A file that follows a strict form specified by penEasy, it gives information about the simulation setup. It is used as input for the PENELOPE simulation.

5.2. Functional Requirements

5.2.1. User Requirements

(i) Users shall be able to enter configuration details for the material to be tested and the geometry specifications.

(ii) Users shall be able to get an output file and energy deposition plot.

(iii) Users shall be able to create a material file.

(iv) Users shall be able to provide the ID or compound information to create a material file.

(v) Users shall be able to create the simulation configuration file.

5.3. Non-Functional Requirements

(i) ODYSSEUS shall undergo rigorous validation and verification testing to ensure its accuracy and reliability. It should be compared with Monte Carlo simulations to ensure that its results match those obtained through traditional methods.

(ii) ODYSSEUS shall allow for customization of input parameters and output formats to suit the needs of different users and applications.

(iii) ODYSSEUS shall be able to handle errors gracefully and provide clear error messages to the user if inputs are invalid or if an error occurs during the simulation or machine learning process.

(iv) ODYSSEUS shall be able to provide results quickly and efficiently. It should be optimized to run on modern hardware, such as GPUs, to minimize computation time.

(v) ODYSSEUS shall come with clear documentation that outlines its functionality, limitations, and potential use cases. It should also provide instructions on how to use the interface and interpret the results.

6. DESIGN

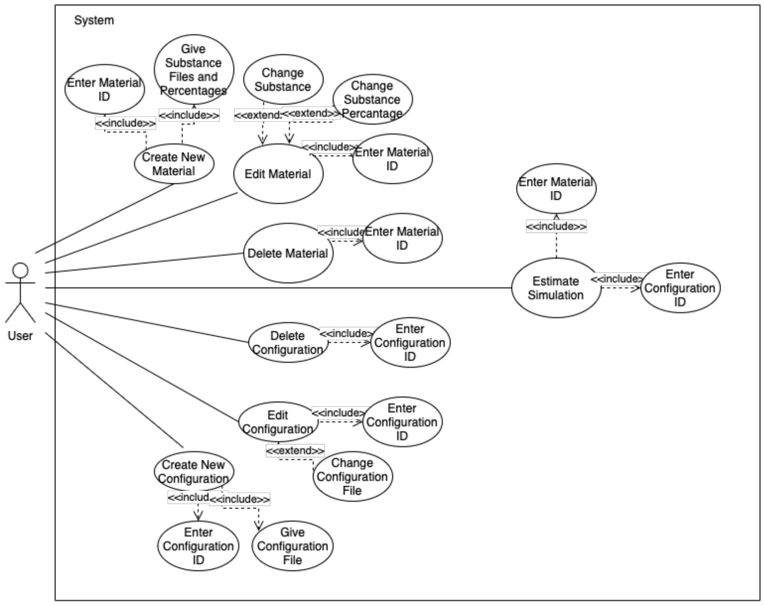


Figure 6.1. Use Case Diagram

In order to obtain reliable simulation data for later usage in our training model, we are currently working to automate the simulation process. We are also investigating machine/deep learning algorithms in order to discover the most suitable model for our project. For the second term, we intend to begin deploying and implementing our tool. Thus, we haven't decided on the structure and haven't finished creating all the diagrams. First, we must determine which variables are most important to our project. Diagrams are not required at this point of our project because we will start developing our tool after gathering enough data to train an ANN model.

7. IMPLEMENTATION AND TESTING

7.1. Implementation

ODYSSEUS will be a two-semester project, therefore we have divided the planning into two periods. In the first period, our goal is to run the PENELOPE simulation and by doing so, generate data as much as we can to use with deep learning algorithms. In the meantime, we will continue reviewing the literature and learn more information about the possible ANN structures. In the next period, we will be building an ANN structure and making use of deep learning algorithms and we will train the ANN with the simulation data we have generated this semester.

So far, we have completed setting up and using PENELOPE and PenEasy. We have also managed to run nearly 2500 simulations on the HPC cluster provided by Bogazici University Computer Engineering Department. We have learnt how to use Fortran, which is essential to run the simulations, on this cluster using rootless docker. We have also documented a tutorial on using rootless docker to help others. This has allowed us to generate large amounts of data for a wide range of materials and thicknesses, which will be valuable for training your ANN model in the second semester.

In terms of the simulations we have done, we have achieved to the number of simulations we have planned before that includes various materials and thicknesses to be inspected. We are working on determining the input features for our ANN. We also plan to run the simulations for other materials with different ratios of polymers and material thickness configurations as well(Please see Figure 2.1).

Based on the research we have done on Artificial Neural Networks, we decided to follow supervised training for our model. In supervised learning inputs and outputs are provided and the outputs for the test data is compared with the correct outputs [5]. We will separate the generated simulation data into training and test data sets. For the training step of the ANN model, we will feed the simulation input variables and energy deposition output values for the experiment setup. After learning step we will test our model will the test data and compare the predicted energy deposition values with the correct values provided by PENELOPE.

A study about the finite element model (FEM), a MC simulation for solid mechanics also mentions the computational cost of Monte Carlo simulations and suggest a recurrent neural network as a solution [6]. We will be exploring and learning more about different types of neural networks to use the most efficient one for our specific task.

7.2. Testing

The simulation output predictions produced by ODYSSEUS will be compared to those produced by PENELOPE in order to assess its correctness. PENELOPE is a well-established Monte Carlo simulation software and is considered to be the benchmark in the field of radiation physics. The simulation results from PENELOPE will serve as the standard for measuring how accurate ODYSSEUS is. For the chosen materials and geometries, it may be said that ODYSSEUS is accurate and can be used in place of time-consuming Monte Carlo simulations if the outputs it produces match the benchmark results from PENELOPE.

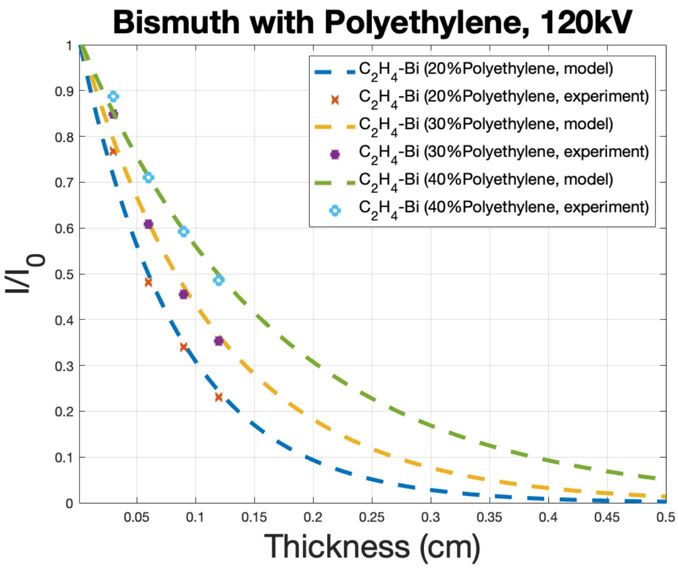
Validation data that was not included in the training phase will be used to test ODYSSEUS. As a result, ODYSSEUS's accuracy will be assessed based on its capacity to anticipate simulation results for brand-new inputs that were not utilized during training. Statistical measurements like root mean square error (RMSE) will be used to assess the effectiveness of ODYSSEUS. If ODYSSEUS has a low root mean square error (RMSE), it may be said that it is a dependable tool for forecasting simulation results.

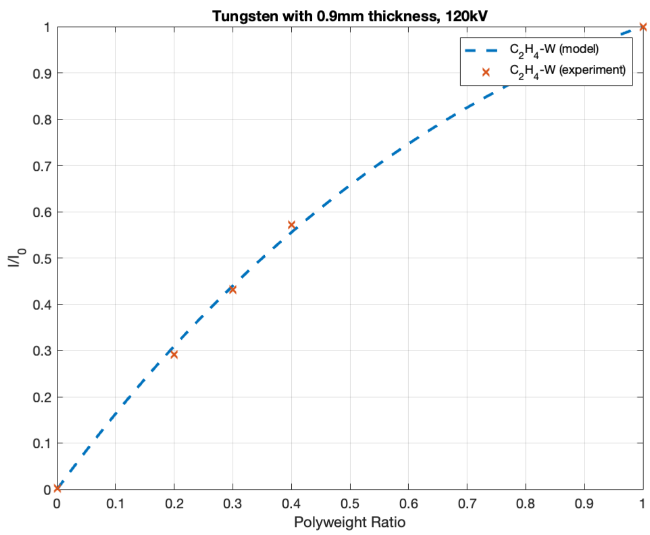
7.3. Deployment

The deployment procedure includes making ODYSSEUS accessible to those who require it for material design jobs. One possible way to utilize the tool is through a graphical user interface (GUI), which lets users enter the required material and geometry parameters and receive the simulation results without having to be familiar with the ANN tool or the underlying Monte Carlo simulations. The GUI can be designed to be user-friendly and straightforward so that users with no prior simulation software expertise can use it. For now, we don't have a strict plan for a possible GUI, but in the second period of our planning, we will determine the deployment process thoroughly.

8. RESULTS

We have completed first part of ODYSSEUS project, which consists of generating simulation data sets to train and test our ANN model for second part. We have generated over 2500 different simulations, confirmed some of their validation with already existing simulation results from other projects. We have plotted results for some of the materials to better understand the relation between radiance attenuation and some input features like thickness and poly weight ratio. Here are two plots that shows the relation:




Tungsten with 0.9mm thickness, 120kV
C_2H_4-W (model)
C_2H_4-W (experiment)
I/I_0
Polyweight Ratio
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

9. CONCLUSION

To sum up, the goal of this project is to create an artificial neural network (ANN) tool that can estimate the results of Monte Carlo simulations for electron and photon transport in arbitrary materials for a broad energy range. For certain materials and geometries that fall under the area of wearable protective materials, the ANN model is anticipated to replace the need for Monte Carlo simulations. We have utilized penEasy to set up and executed simulations on both local PCs and the HPC cluster. We will also create new simulations and gather simulation results for various system configurations.

This project is anticipated to produce a simplified material design procedure that is quicker and less expensive than conventional Monte Carlo simulations. By offering a tool for more effective material design, the created ANN model may significantly advance the field of radiation-protective materials.

Overall, ODYSSEUS offers the chance to investigate artificial neural networks' potential for enhancing the effectiveness and precision of Monte Carlo simulations, as well as to contribute to the creation of radiation-protective materials.

You can find our repository using the following link: `https://github.com/mumcusena/ODYSSEUS\_simulations`

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