Mesh RNUCS Progress Report

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Contents

List of Tables

List of Figures

1 Introduction

This report covers the work performed at UW in efforts to create a mesh rnucs worflow.

During operation of accelerator based system, like the Spallation Neutron Source (SNS), the nuclear reactions happening in the system produce high energy neutrons that penetrate deep into the components of the system. The materials of the components become activated from the neutron irradiation and release high energy photons that persists even after shutdown. These photons can negatively impact the health of a human body. During maintenance, personnel come in close contact with these components, therefore it becomes important to quantify the dose rates from these photons. Quantification of these dose rates in nuclear systems have traditionally been performed computationally and workflows exist to aid the calculation. A common way to solve these problems is by coupling the neutron transport and photon transport calculations using activation analysis, known as the Rigorous 2 Step (R2S) method. The R2S method has been implemented at UW as an automated workflow with fidelity determined by a superimposed mesh, and has been added to the Python for Nuclear Engineers (PyNE) package. The UW-R2S capabilities only extend to energies in the fusion system region (20 MeV) and future work need to be performed to extend the capabilities to accelerator systems. In higher energy regions such as those encountered in accelerator-based systems, R2S workflows have been developed to be able to perform a complete analysis in these systems. One such workflow relies on a radionuclide inventory tally (RNUCS) implemented in MCNPX to obtain reaction rates across the full energy spectrum. These results are used during the activation step, producing photon sources, but with fidelity limited to individual geometric volumes.

2 Background

2.1 Nuclear Inventory Analysis

When a material is irradiated a variety of reactions can happen which can lead to production of radionuclides. These radionuclides persist even after a device is shutdown. A nuclear inventory must be known in order to quantify the photon emission density as a function of time. The production and destruction of nuclides can be modeled mathematically.

The rate in which nuclide i undergoes a reaction is given by equation 1

$$P_{i\to j,reaction} = \int_{E_n} \sigma_{i\to j}(E_n)\phi_n dE_n \tag{1}$$

where $\sigma_{i\to j}(E_n)$ is the microscopic cross section for the reaction that transforms nuclide i into j, and $\phi_n(E_n)$ is the neutron flux for energy E_n.

The production rate constant for the decay process is given by equation 2

$$P_{i\to j,decay} = \lambda_i b_{i\to j} \tag{2}$$

where λ_i is the decay constant and $b_{i\to j}$ is the branching ratio.

The total rate is given by equation 3

$$P_{i\rightarrow j,decay} = \lambda_i b_{i\rightarrow j} \quad (3)$$

2.2 General Shutdown Dose Rate Workflow

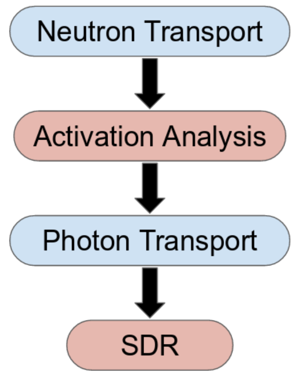


Figure 1: General shutdown dose rate workflow

2.3 Shutdown Dose Rate Workflow for High Energy Systems

The current SDR workflow is seen in Figure 2

3 Implementation

The numerical experiments conducted in this work required the development of a collection of scripts and patches that ultimately form the Shutdown Dose Rate workflow as seen in Figure 3

3.1 MCNP Patch

The first step in the rnucs R2S workflow is the neutron transport step therefore a change in the MCNP source code was necessary in order to collect radionuclide information in a mesh. These MCNP changes were recorded in a patch file. This file should be applied directly to MCNP6.1 after a DAGMC patch has been applied. This patch DAG-MCNP6.1 will output a file with the name r_mesh which stores radionuclide information per voxel.

3.2 Activation Script

A python script was created to collect mesh rnucs information from the r_mesh file, flux information from a meshtal file, and material information from a material laden CAD geometry. This collected information is then written out in the correct format and in the right files that can be read by the activation software CINDER90.

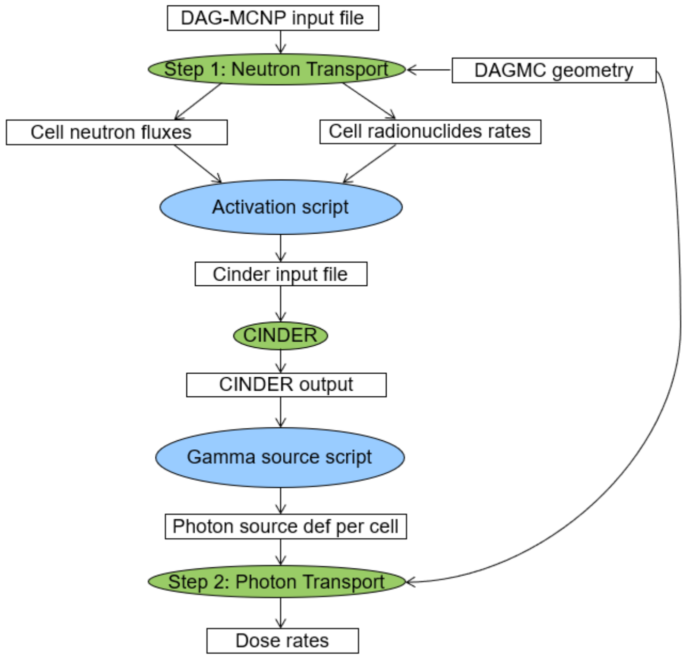


Figure 2: Current shut down dose rate workflow for Accelerator systems as used by ORNL

The original perl activation script is used to read a keyword ”mesh” and call the python script mentioned above, write an input file for each region/voxel and run the CINDER90 and TABCODE software.

4 Analysis

In order to asses the correct progress of the rnucs-mesh workflow, a few analysis were performed on two toy problems.

4.1 Problem Description

Two toy problems were identified to asses the correctness of the rnuc-mesh workflow. Toy problem 1 (Figure **??**) consists of a mercury box with geometrical specifications as listed in Table 1. Toy problem 2 (Figure **??**) consists of a mercury box surrounded by a steel box. The specifications can be found in Table 1

All problems were run with a 1 GeV proton source in the z direction and with 1E6 particles.

Six geometries were created, three for each toy problem. The first geometry was built as described above, the second geometry was split into 8 equal cells and the last one was split 64 equal cells. Splitting toy problem 2 into 8 equal cells required that the materials be mixed in a 3:1 ratio

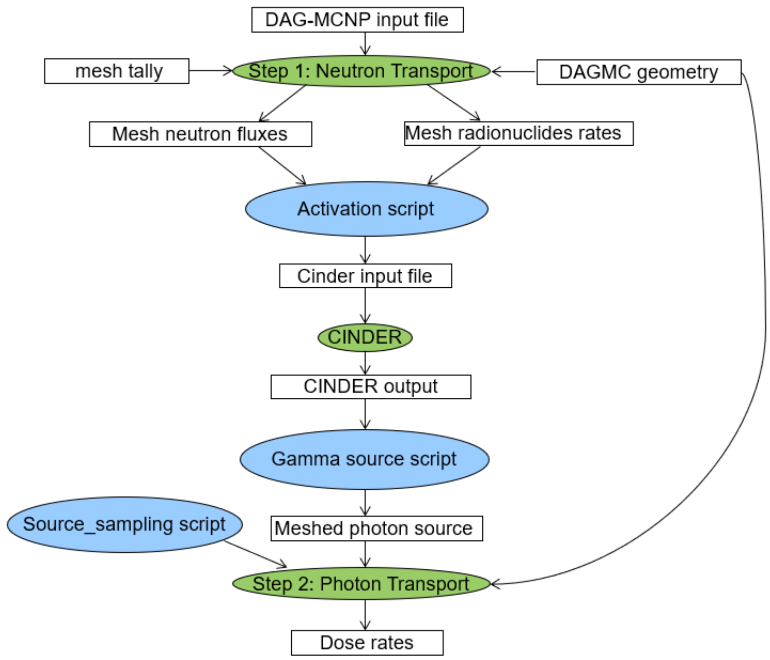


Figure 3: Mesh RNUCS Workflow

Geometry	X position (cm)	Y position (cm)	Z position (cm)
Toy problem I	-11, 11	-22, 22	-93, 93
Toy problem II	-22, 22	-44, 44	-186, 186

Table 1: Toy problems dimensions

4.2 Workflow to Photon Emissions

In oder to generate the spectrum file, the following steps were carried out:

- MCNP run
- Generation of

The following runs were performed:

- rnucs on cells
- 1x1x1 mesh
- 2x2x2 mesh
- 4x4x4 mesh
- 2x2x2 split

- 4x4x4 split

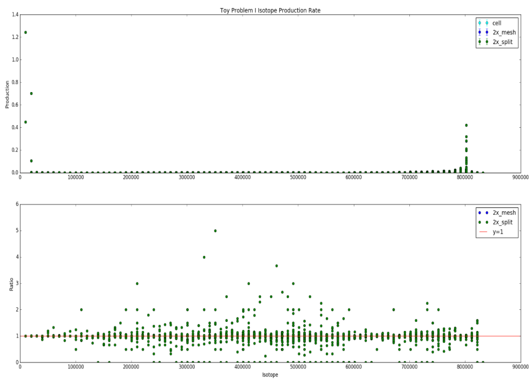
Each mesh covered the entire geometry and was uniformly distributed. Splitting toy problem II into 8 equal parts required the mixed material to be created. The mixed material was 3:1 ratio of steel and mercury.

4.3 Activation

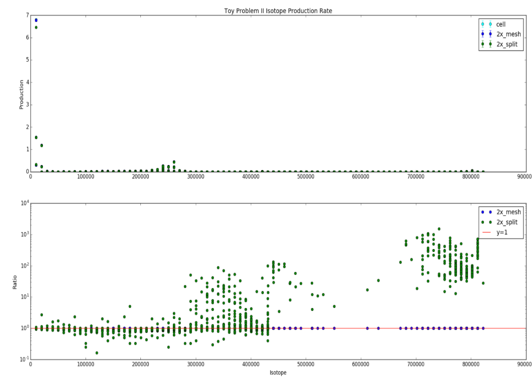
An activation calculation was done for each run for a set of irradiation history.

5 Results

A comparison of the radionuclide production between a cell rnucs, meshed rnucs, and geometry split rnucs for Toy Problem I and Toy problem II are shown in Figures 4a and 4b respectively.



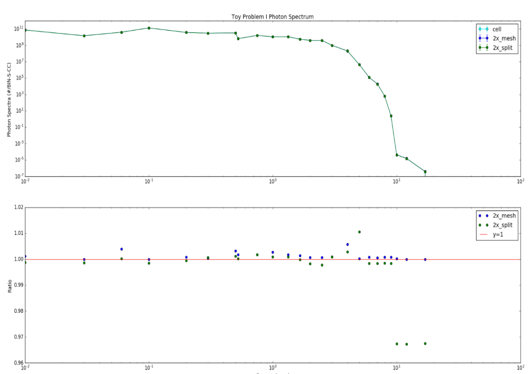
(a) Toy problem I



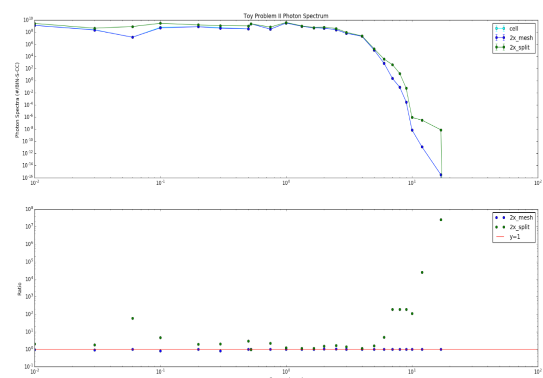
(b) Toy problem II

Figure 4: Radionuclide production for cell, meshed and split geometries

Figures 5a and 5b show a similar comparison for the photon spectrum.



(a) Toy problem I



(b) Toy problem II

Figure 5: Photon Spectrum at 1hr after shutdown

Figures 4 and 5 suggest that the splitting the geometries differs the most from the original rnucs workflow. In this particular case, splitting the geometry into 8 equal parts for Toy problem II required material mixing. This is likely to show in the large discrepancy between the cell case and the split case.

Another important comparison is that of the cell rnucs with the progression of the mesh rnucs. Figure 6 shows the order of the voxels used in Figure 7.

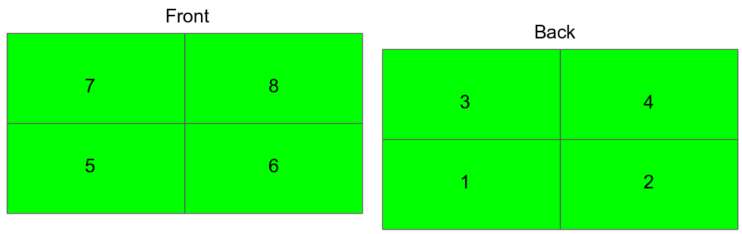
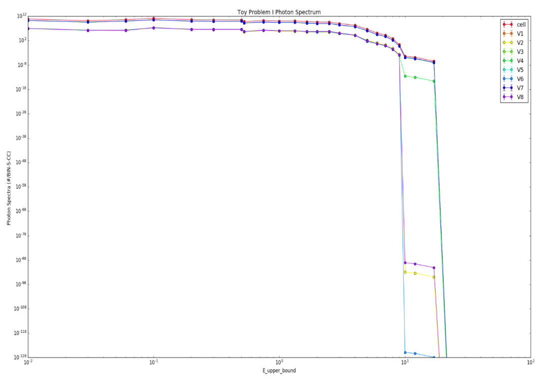
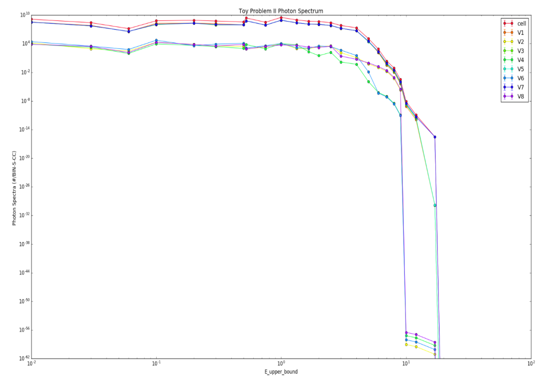


Figure 6: Voxel configuration



(a) Toy problem I



(b) Toy problem II

Figure 7: Photon Spectrum at 1hr after shutdown for each voxel in a 2x2x2 mesh

In Figure 7 there are three distinct set of the lines, the first one is the one for the cell, the second set belong to voxels 1, 3, 5, and 7, and the last group belongs to voxels 2, 4, 6, and 8. Voxels 1, 3, 5, and 7 have greater photon emission than the voxels 2, 4, 6, and 8. This is expected as the source is to the left of the geometry. Having a mesh gives more spatial definition which is useful for large geometric cells.