

Model Inputs and Outputs



Figure 1) Photograph of HF-ADNeF target room.

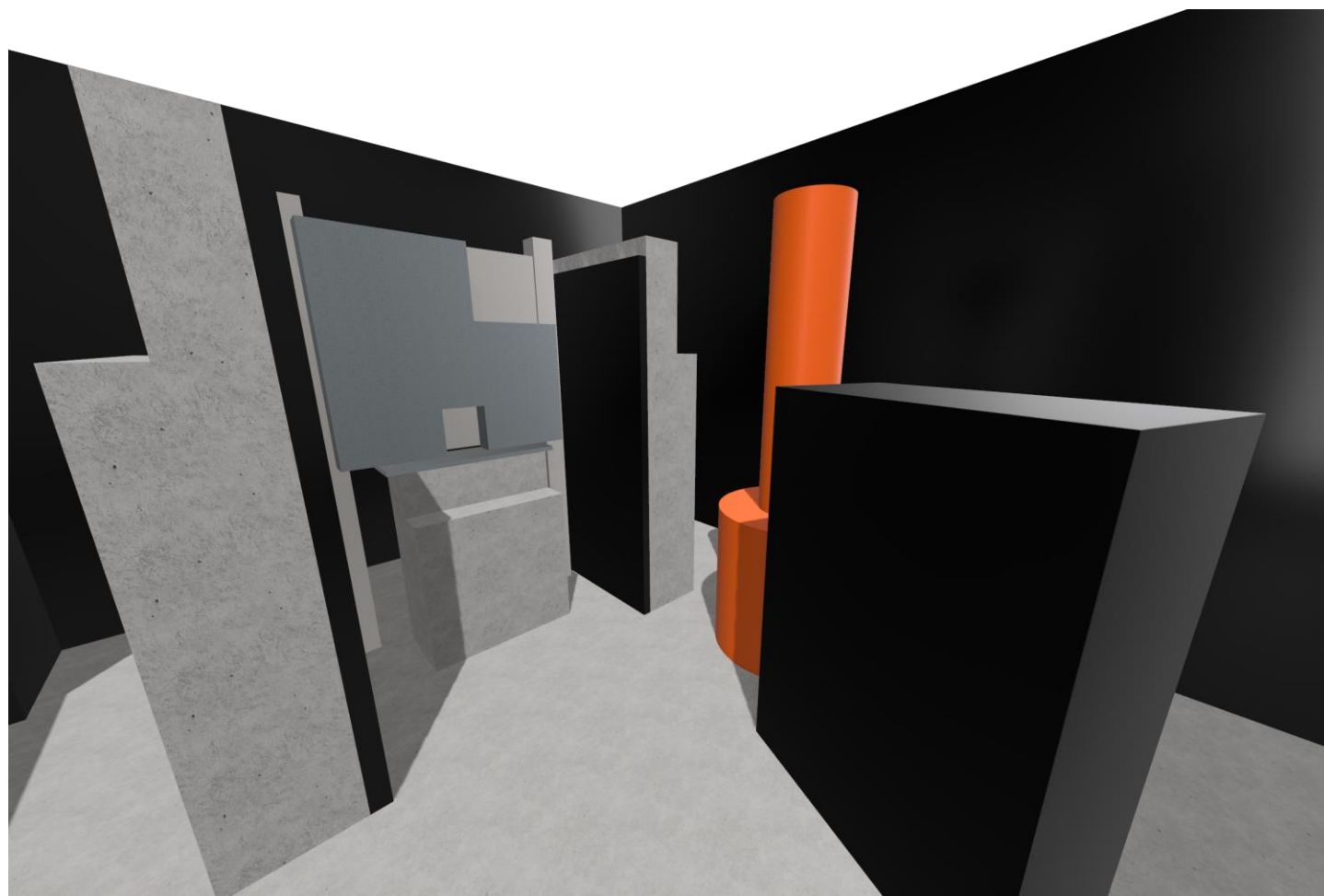


Figure 2) 3D CAD model of HF-ADNeF target room.

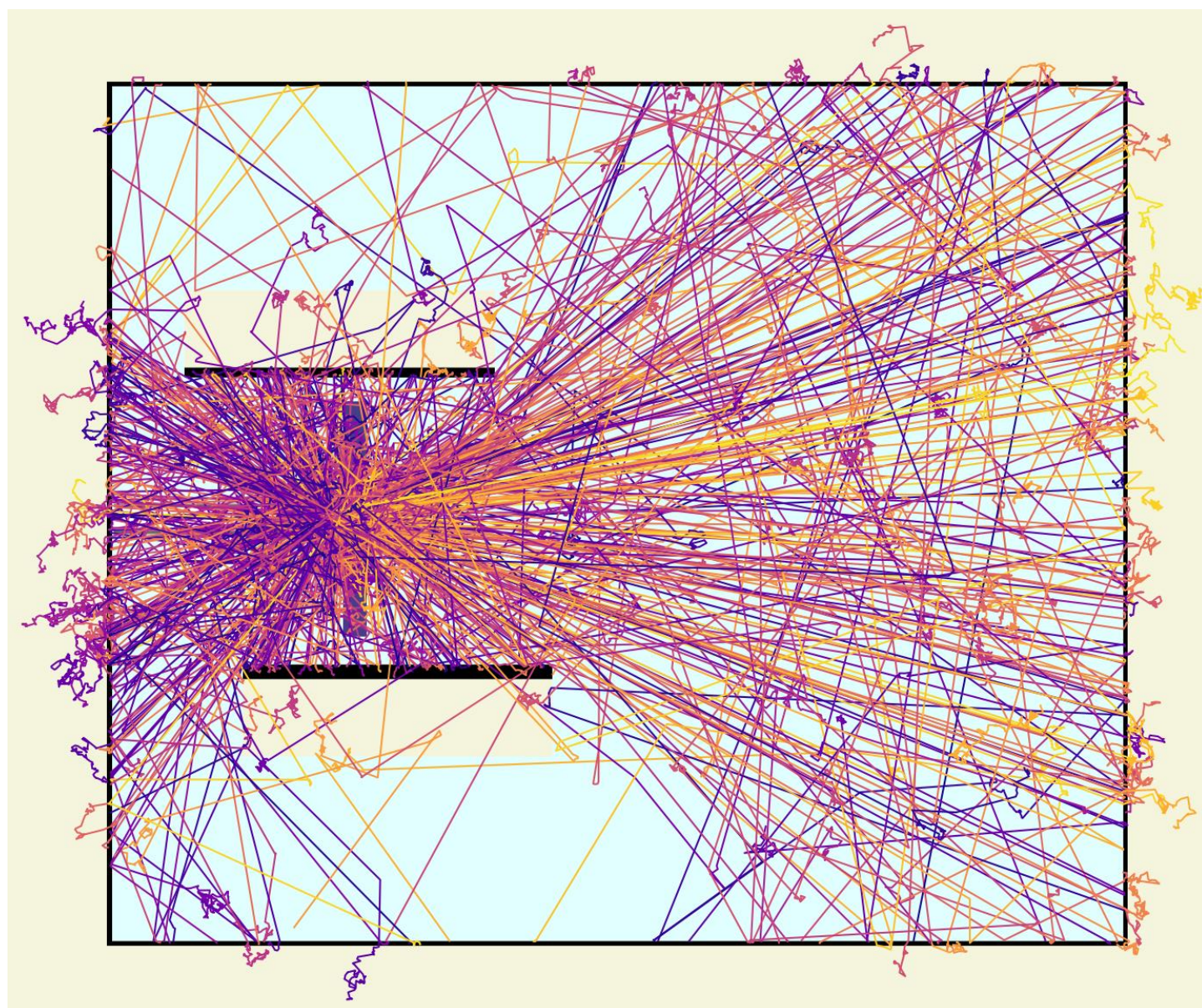


Figure 3) Top-down view of neutron tracks, colour coded by initial neutron energy.

Geometry:

- A 3D model of the target room has been developed in OpenMC and can be imported as a Python package.
- Activation foils, moderating materials and more can be added using functions to prevent boundary clashes.

Starting Neutron Information:

- A C++ source file is defined based on MCNP input cards, using data from Minsky et al, for each proton energy.
- A neutron energy is first sampled via linear interpolation.
- Based on this neutron energy, the relevant angular distribution is sampled for the lab emission angle.

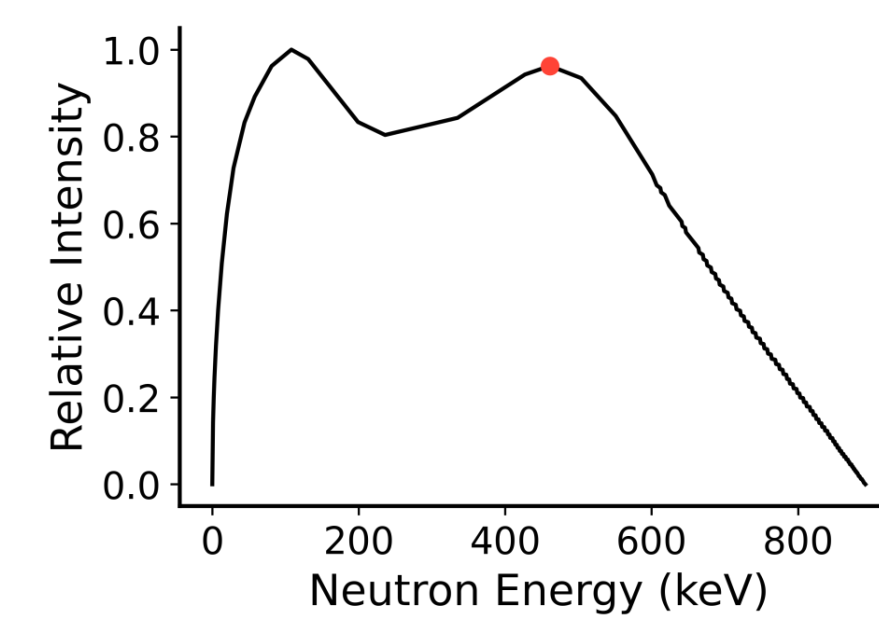


Figure 2) Neutron energy distribution for 2.6 MeV protons incident on target.

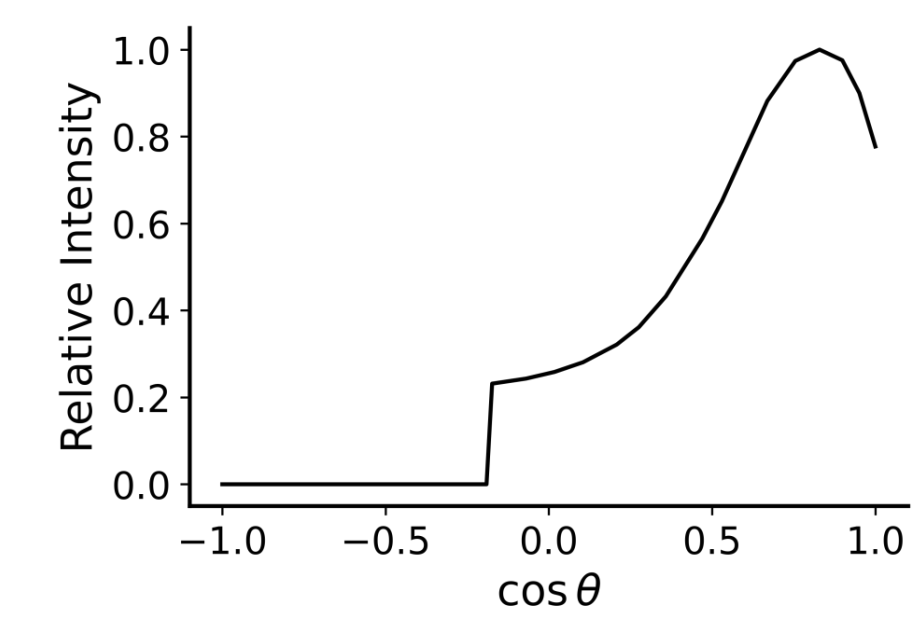


Figure 3) Angular distribution for 461 keV neutron sampled in figure 2.

Neutron Tracks:

- A **track file** contains neutron position and energy information at each step.
- This allows for validation and of the **neutron transport** in the problem.

Tally Normalisation:

- Tallies such as flux and (n,γ) are output per source particle.
- Multiplying by a **source strength** term gives the number of neutrons per mC of proton beam, also given by Minsky et al.
- A final result is achieved by multiplying by proton current.

OpenMC simulations of the UoB HF-ADNeF for Medical Isotope Production

M Conroy^{1,2}, T Price¹, M Freer¹, B Slingsby², R Mills², L Capponi², Tz Kokolova¹, C Wheldon¹

¹School of Physics and Astronomy, University of Birmingham, UK

²National Nuclear Laboratory, Warrington, UK



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Introduction

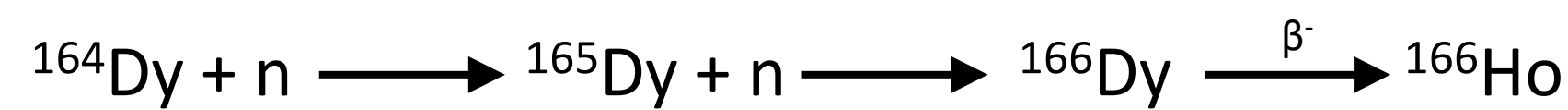
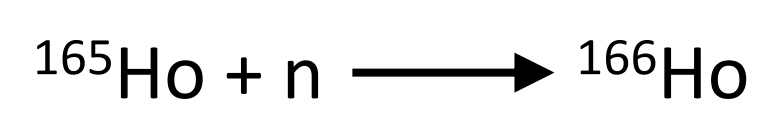
The **high-flux accelerator driven neutron facility** (HF-ADNeF) at the University of Birmingham can produce neutron fluxes of up to $10^{12} \text{ n s}^{-1} \text{ cm}^{-2}$ [1].

An **OpenMC** simulation has been produced to investigate the possibility of **producing novel medical isotopes** at this facility, under various irradiation conditions [2].

Holmium-166 is an exciting medical isotope, emitting both **beta** and **gamma** (80.6 keV) radiation, making it suitable for both **therapy** and **imaging** [3].

Holmium-166 Production

Production of ^{166}Ho ($t_{1/2} = 26.6$ hours) can be via **two routes** [3]:



The first is simple and produces **high yields**, since natural holmium is 100% ^{165}Ho .

Although the second route requires double neutron capture, the **cross sections** for both reactions are very high.

Since ^{166}Dy has an 81.5 hour half-life, a **$^{166}\text{Dy}/^{166}\text{Ho}$ generator** can be produced, which is more convenient.

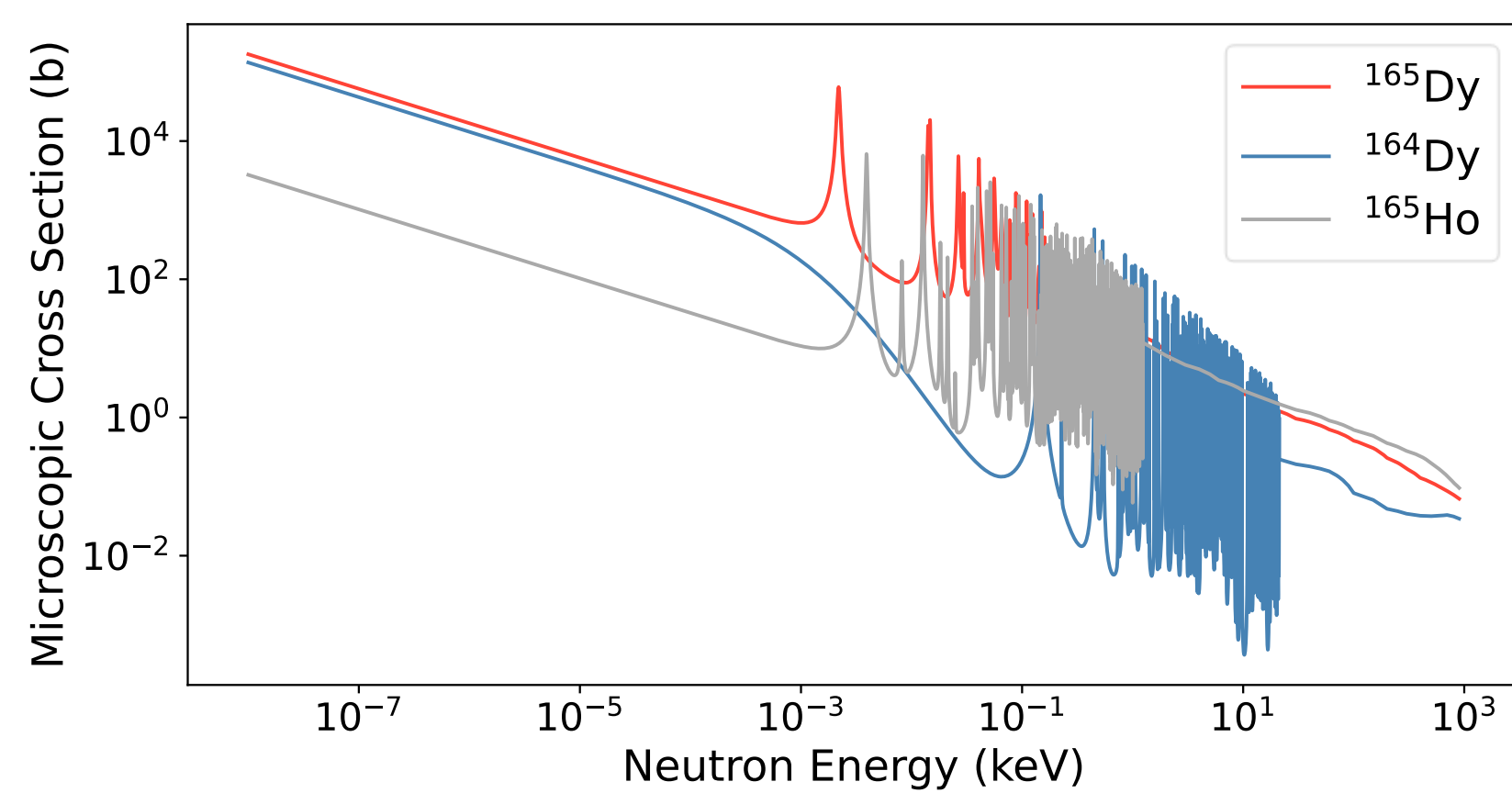


Figure 6) TENDL-2019 cross sections of (n,γ) in ^{165}Ho , ^{164}Dy and ^{165}Dy .

Model Overview

Geometry

- A **3D model** of the HF-ADNeF target room has been developed in **OpenMC** and can be imported as a **Python package**.
- Activation foils, moderating materials and more can be added using **functions** to prevent boundary clashes.

Starting Neutron Information

- A **source file** is defined for each **proton energy**, based on MCNP input cards [4].
- A **neutron energy** is first sampled from an **energy distribution** via **linear interpolation**.
- Based on this neutron energy, the relevant **angular distribution** is sampled for the **lab emission angle**.



Figure 1) Photograph of HF-ADNeF target room.

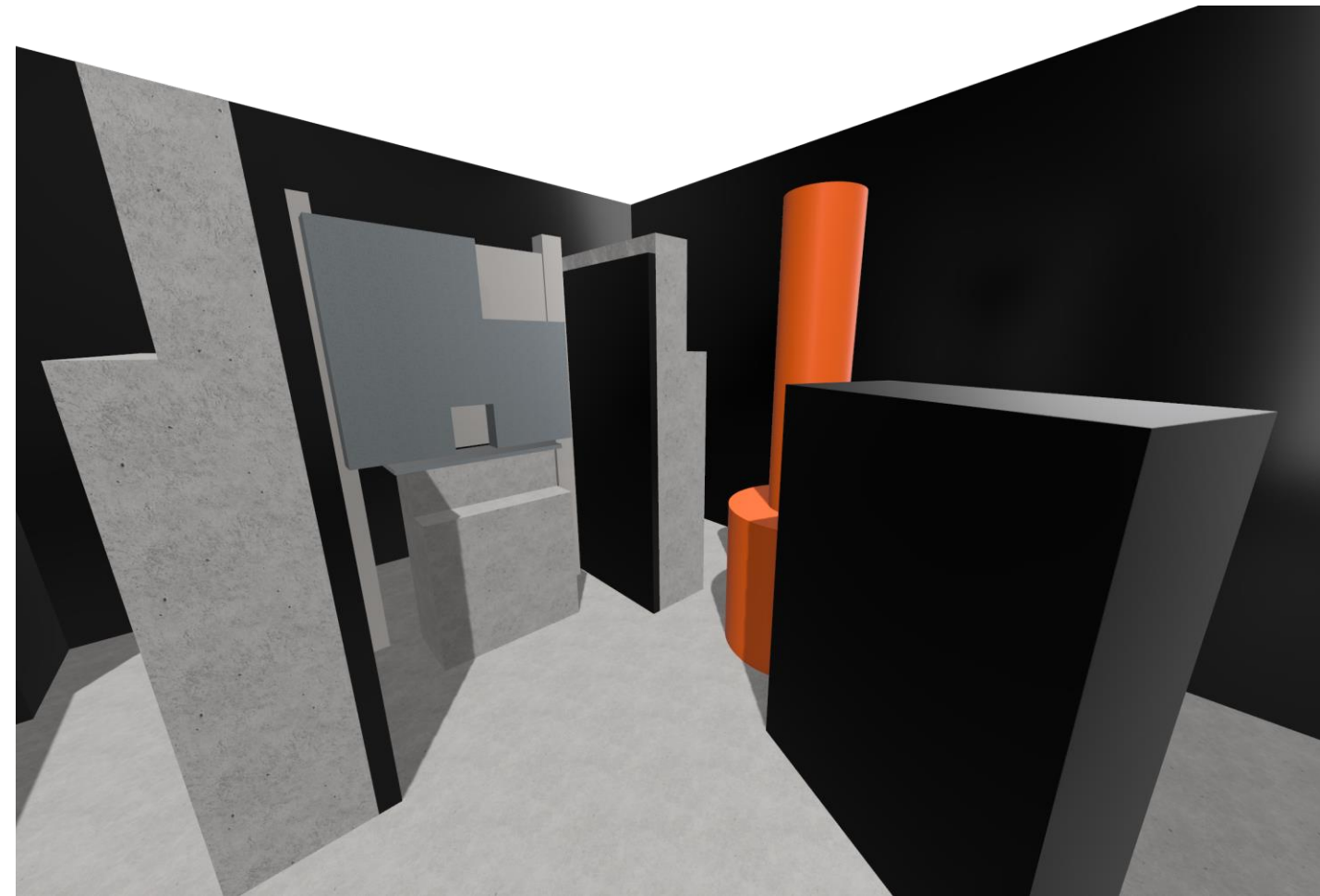


Figure 2) 3D CAD model of HF-ADNeF target room.

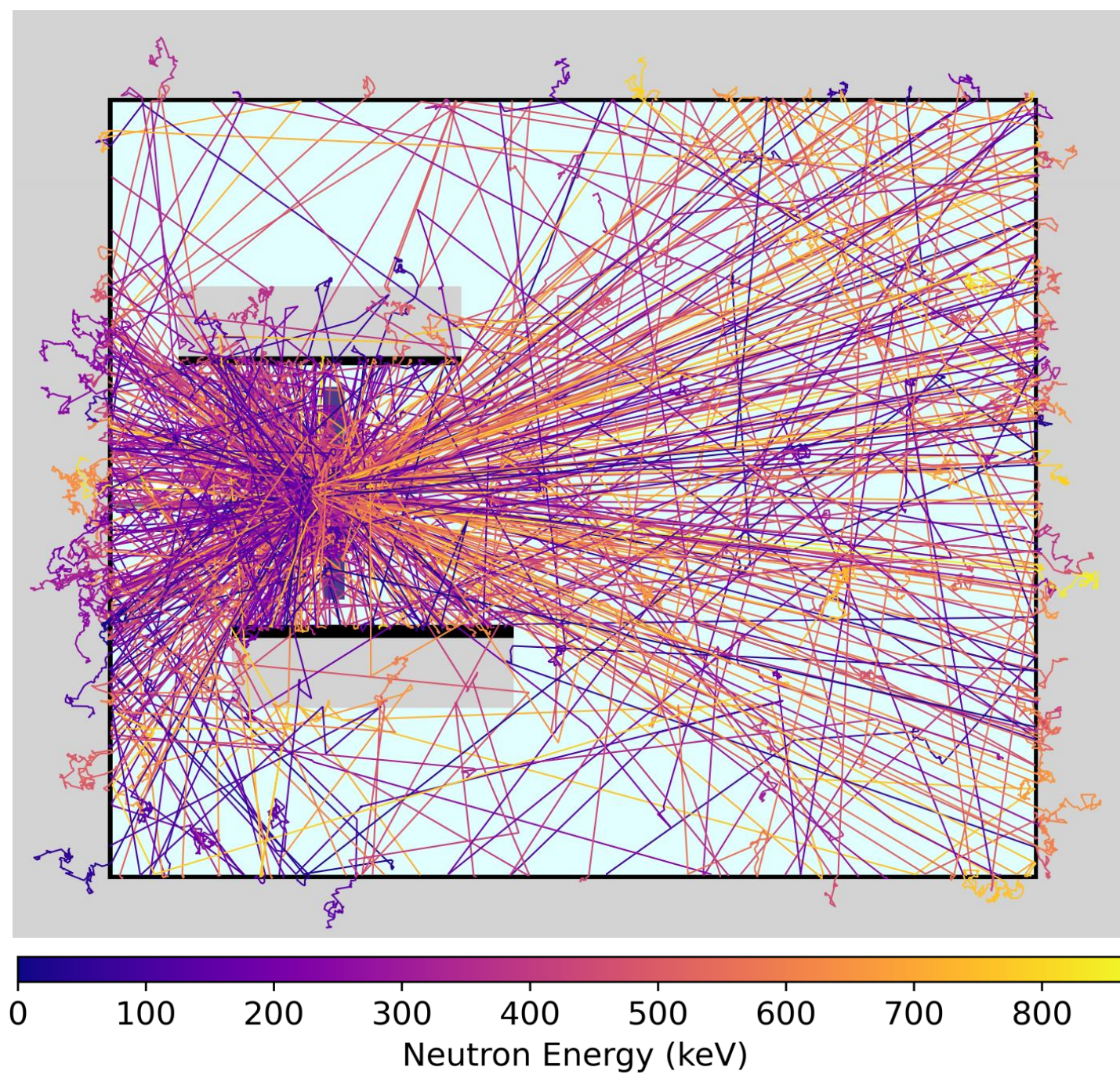


Figure 3) Top-down view of neutron tracks in target room, colour coded by initial neutron energy.

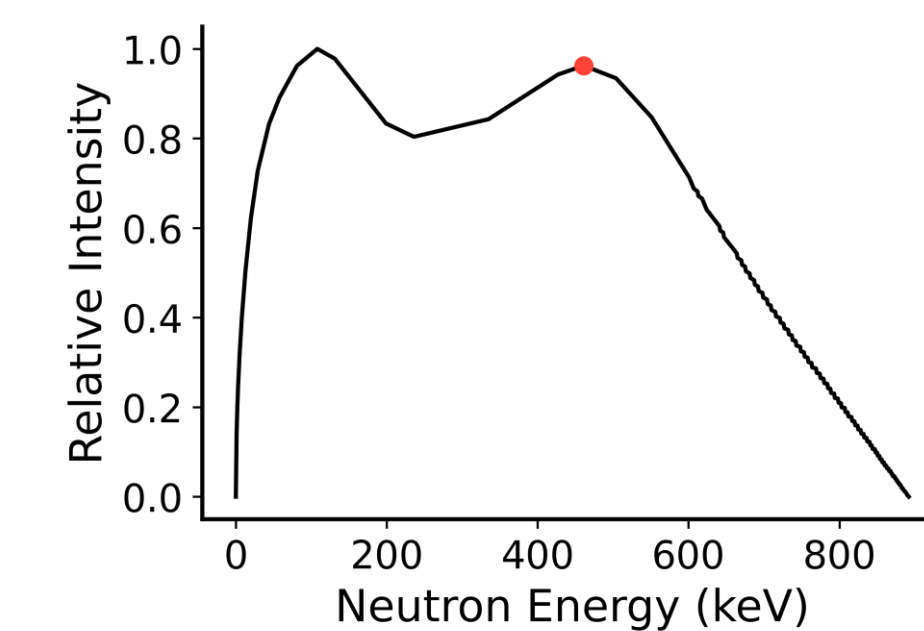


Figure 4) Neutron energy distribution for 2.6 MeV protons incident on target.

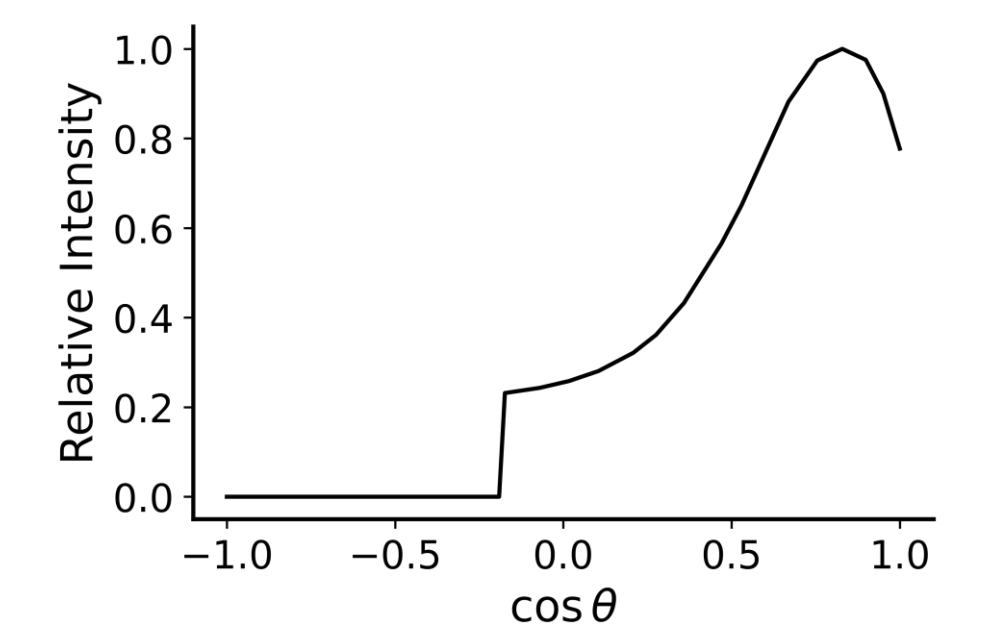


Figure 5) Angular distribution for 461 keV neutron sampled in Figure 4.

Neutron Tracks

- A **track file** contains position and energy information at each step.
- This allows for validation of the neutron transport in the problem.

Tally Normalisation

- Tallies such as **flux** and **(n,γ)** are output per source particle.
- Multiplying by a **source strength** term gives the number of neutrons per mC of proton beam at a given energy, based on theoretical yield.

Activity Calculations

The irradiation of a **natural holmium** foil was **simulated**, consisting of 100% ^{165}Ho .

The **normalised (n,γ)** tally within the foil gives the **reaction rate**, R , of ^{166}Ho production.

The **activity** of ^{166}Ho at a given time, t , can then be calculated for a desired irradiation time, t_{irr} ,

$$A = R(1 - e^{-\lambda t_{irr}})e^{-\lambda t}.$$

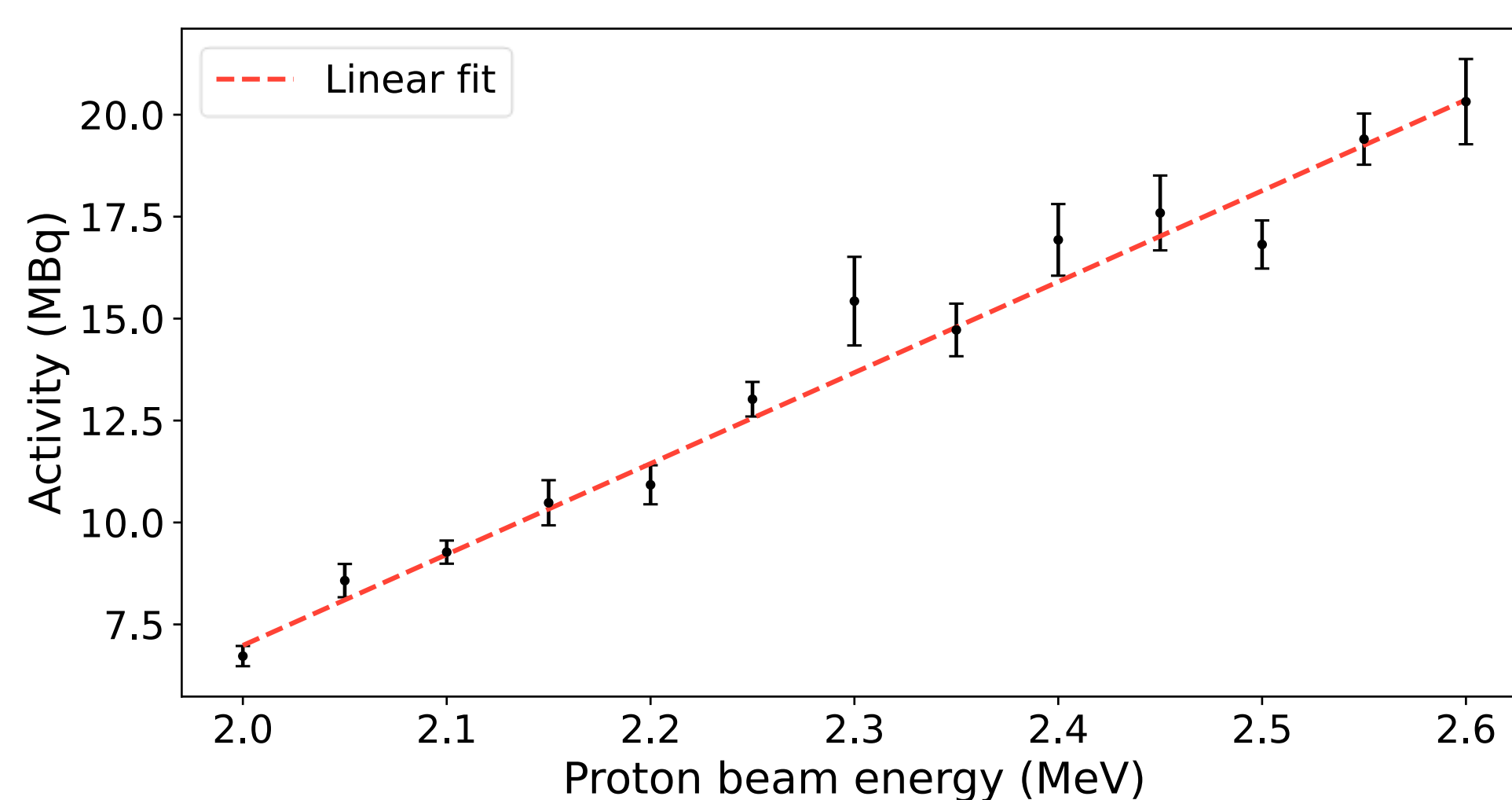


Figure 8) Predicted activities of ^{166}Ho from irradiation of natural Ho foil at fluxes from increasing proton energy at HF-ADNeF. Errors are statistical.

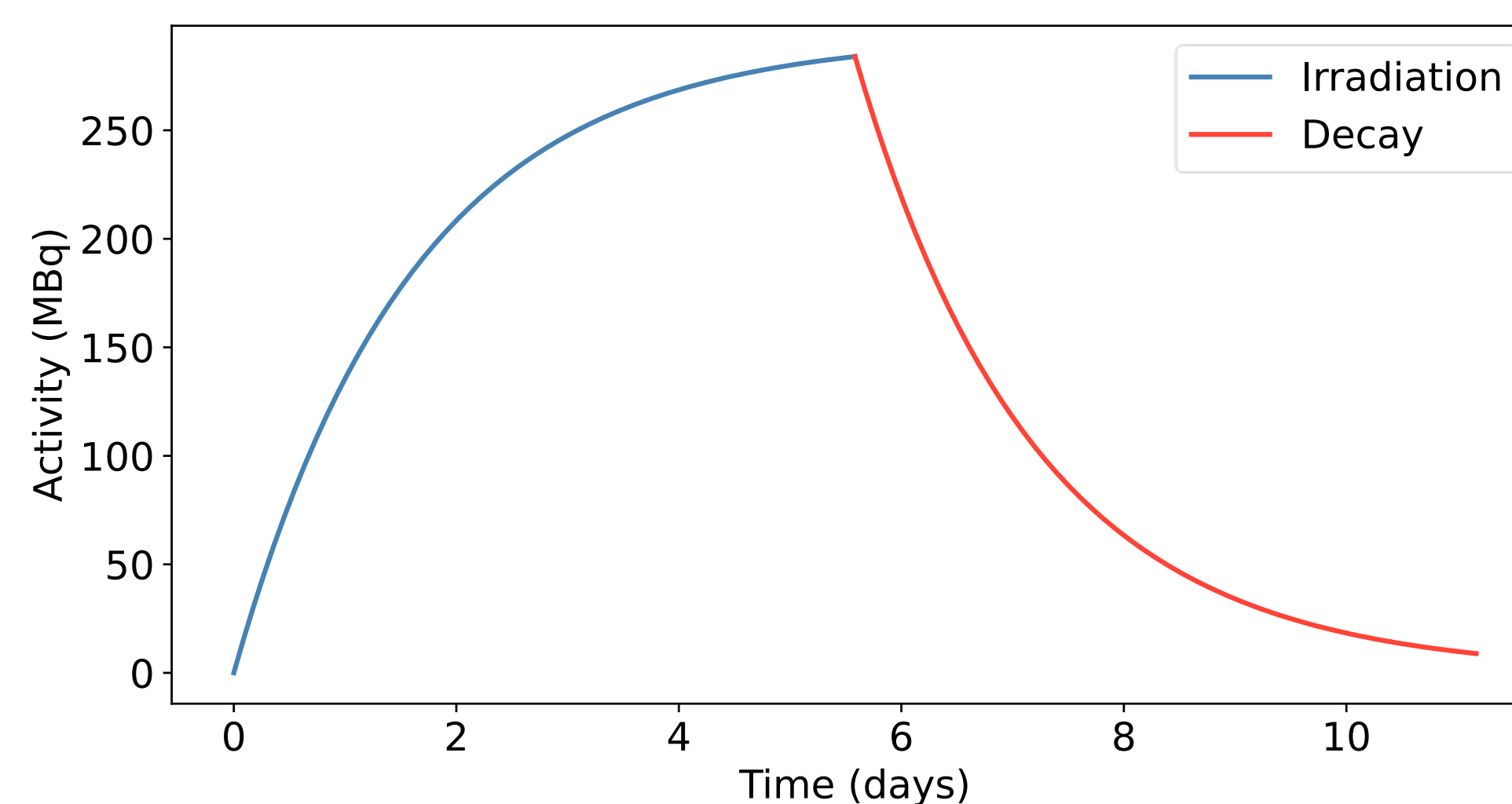


Figure 7) Activity of a natural holmium foil during and after neutron irradiation.

Reaction rates were calculated at **increasing proton energies**, resulting in different neutron yields and flux profiles.

Activities were calculated for **3-hour irradiations** at proton currents of **34 mA**.

A **linear trend** reflects the increase in neutron flux with proton energy [1].

Experimental Work

Both natural **holmium** and **dysprosium** foils were irradiated at HF-ADNeF.

Activation foils were also irradiated for simulation benchmarking.

Gamma spectroscopy was performed to analyse the activity of ^{166}Ho present in the foils.

Preliminary results show an **order of magnitude agreement** between simulated and measured activities.

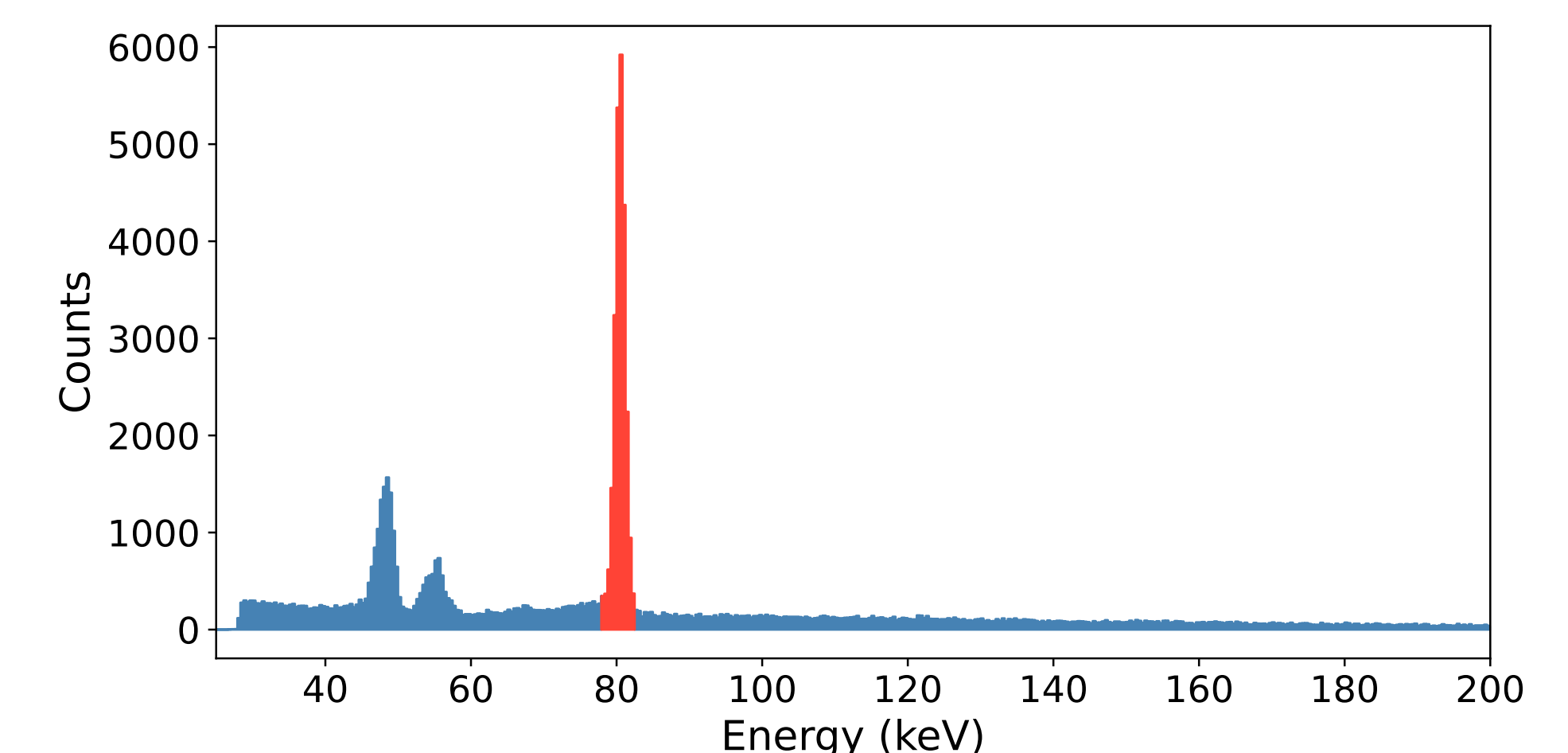


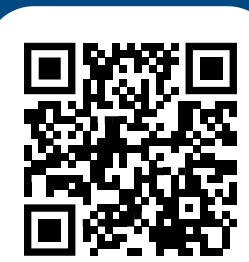
Figure 10) Spectrum of activated Ho foil taken on HPGe detector, showing 80.6 keV peak from ^{166}Ho decay.



Figure 9) MnAl (left) and Ho (right) foil attached to holder to be irradiated.

Acknowledgements

This work was funded by the Hawkesworth fund, University of Birmingham and NNL's Medical Radionuclide Science core science theme.



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Conclusion and Outlook

- An OpenMC model has been created to facilitate activity calculations at HF-ADNeF.
- Predicted activities agree with preliminary experimental results to an order of magnitude.
- Code will be developed to allow (2n,γ) calculations.
- Future comparisons will be made to MCNP and other codes, as well as more experimental data.

References

- A. D. Brooks, Neutron Beams at Birmingham: HF-ADNeF, Poster IOP Joint APP, HEPP and NP conference (2024)
- P. K. Romano et al., OpenMC: A State-of-the-Art Monte Carlo Code for Research and Development, Ann. Nucl. Energy, 82, 90-97 (2015)
- Nienke et al., The various therapeutic applications of the medical isotope holmium-166: a narrative review. EJNMMI Radiopharmacy and Chemistry, [online] 4(1) (2019)
- D. M. Minsky, AB-BNCT beam shaping assembly based on $^7\text{Li}(p,n)^7\text{Be}$ reaction optimization, Appl. Rad. and Isotopes, 69, 12 (2011)

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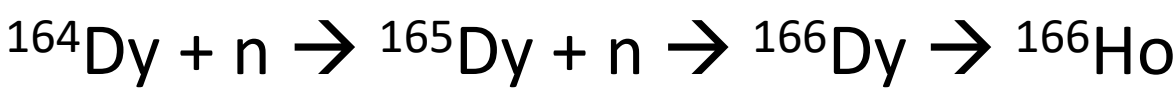
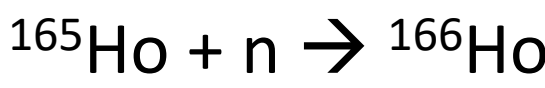
The **high-flux accelerator driven neutron facility** (HF-ADNeF) at the University of Birmingham can produce neutron fluxes of up to **$10^{12} \text{ n s}^{-1} \text{ cm}^{-2}$** .

An **OpenMC** simulation has been produced to investigate the possibility of **producing novel medical isotopes** at this facility, under various irradiation conditions.

Holmium-166 is an exciting medical isotope, emitting both **beta** and **gamma** (80.6 keV) radiation, making it suitable for both **therapy** and **imaging**.

Holmium-166 Production

Production of ^{166}Ho can be via two routes:



The first is simple and produces high yields, since natural holmium is 100% ^{165}Ho .

The second route provides a $^{166}\text{Dy}/^{166}\text{Ho}$ generator, facilitating easy isotope separation.

Plot of Ho and Dy cross sections.

Experimental Work

Both natural **holmium** and **dysprosium** foils were irradiated at HF-ADNeF.

Activation foils were also irradiated for simulation benchmarking.

Gamma spectroscopy was performed to analyse the activity of ^{166}Ho present in the foils.

Preliminary results show an order of magnitude agreement between simulated and measured activities.



Figure 4) MnAl (left) and Ho (right) foil attached to holder to be irradiated.

Plot of holmium (and dysprosium) gamma spectrum(a).
Will not show results of gamma spec analysis, just spectra.

Model Inputs and Outputs

Geometry:

A 3D model of the target room has been developed in OpenMC and can be imported as a Python package.

Activation foils, moderating materials and more can be added using functions to prevent boundary clashes.



Figure 1) Side by side comparison between 3D CAD and photograph of target room.

Neutron Tracks:

A **track file** contains neutron position and energy information at each step.

This allows for validation and of the **neutron transport** in the problem.

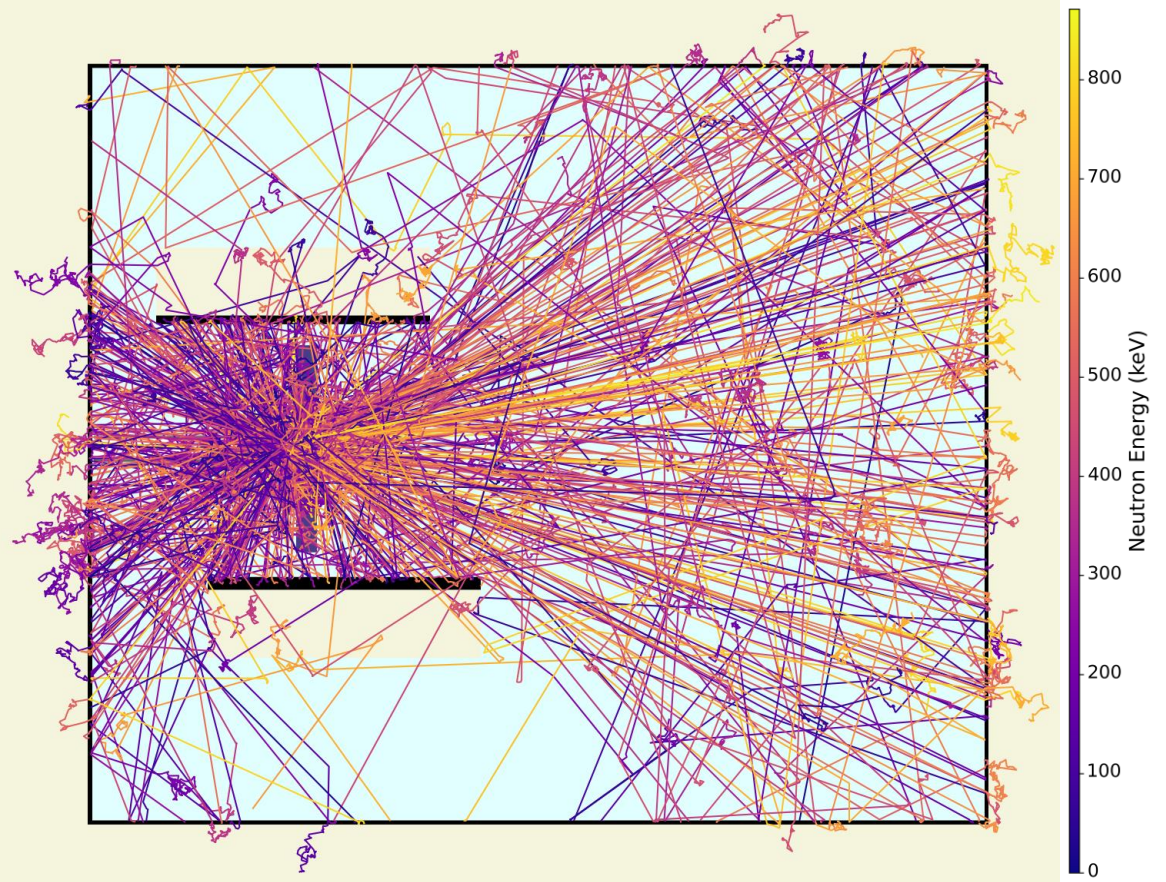


Figure 4) Top-down view of neutron tracks, colour coded by initial neutron energy.

Starting Neutron Information:

A C++ source file is defined based on MCNP input cards, using data from Minsky et al, for each proton energy.

A neutron energy is first sampled via linear interpolation.

Based on this neutron energy, the relevant angular distribution is sampled for the lab emission angle.

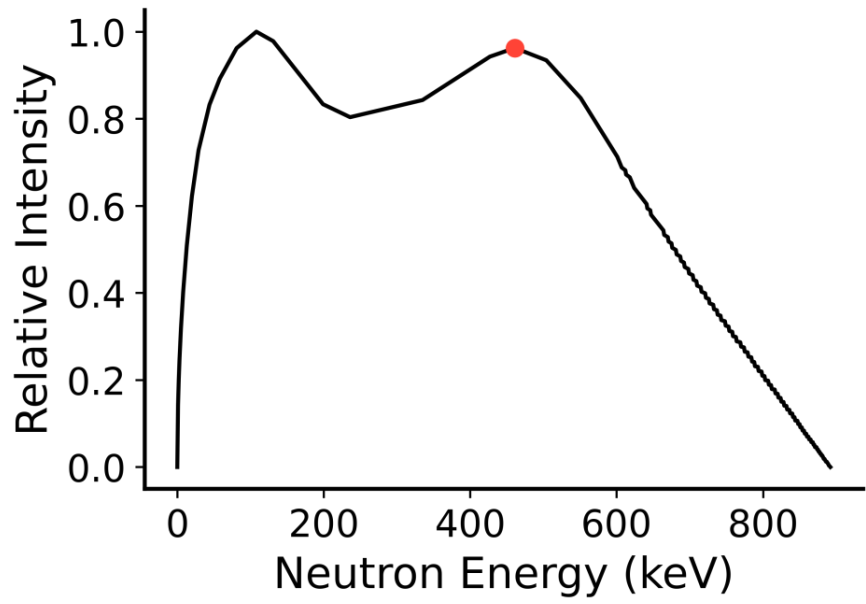


Figure 2) Neutron energy distribution for 2.6 MeV protons incident on target.

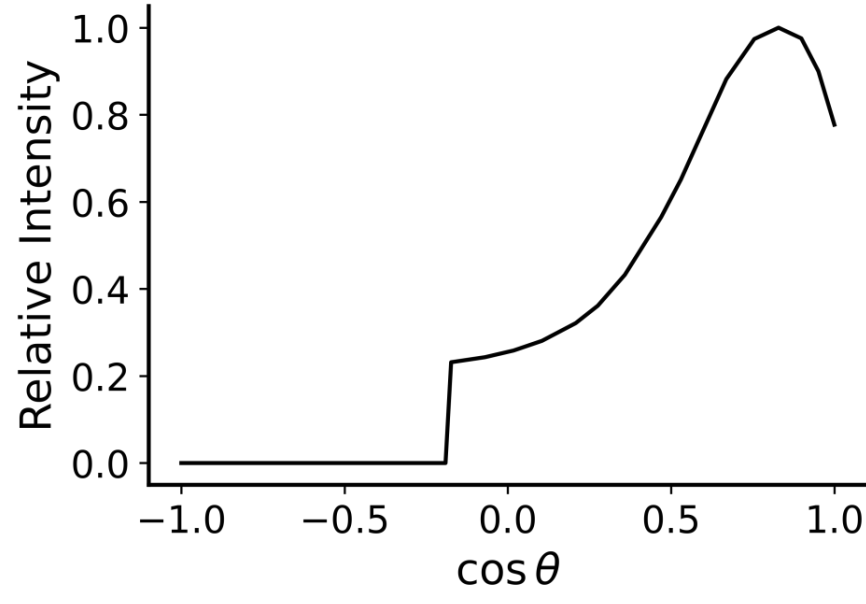


Figure 3) Angular distribution for 461 keV neutron sampled in figure 2.

Tally Normalisation:

Tallies such as flux and (n,γ) are output per source particle.

Multiplying by a **source strength** term gives the number of neutrons per mC of proton beam, also given by Minsky et al.

A final result is achieved by multiplying by proton current.

Activity Calculations

The irradiation of a **natural holmium** foil was **simulated**, consisting of 100% ^{165}Ho .

At present, dysprosium was not considered due to the added complication of **double neutron capture**.

The **normalised (n,γ)** tally within the foil gives the **reaction rate, R**, of ^{166}Ho production.

The **activity** of ^{166}Ho at a given time, t, can then be calculated for a desired irradiation time, t_{irr} ,

$$A = R(1 - e^{-\lambda t_{irr}})e^{-\lambda t}.$$

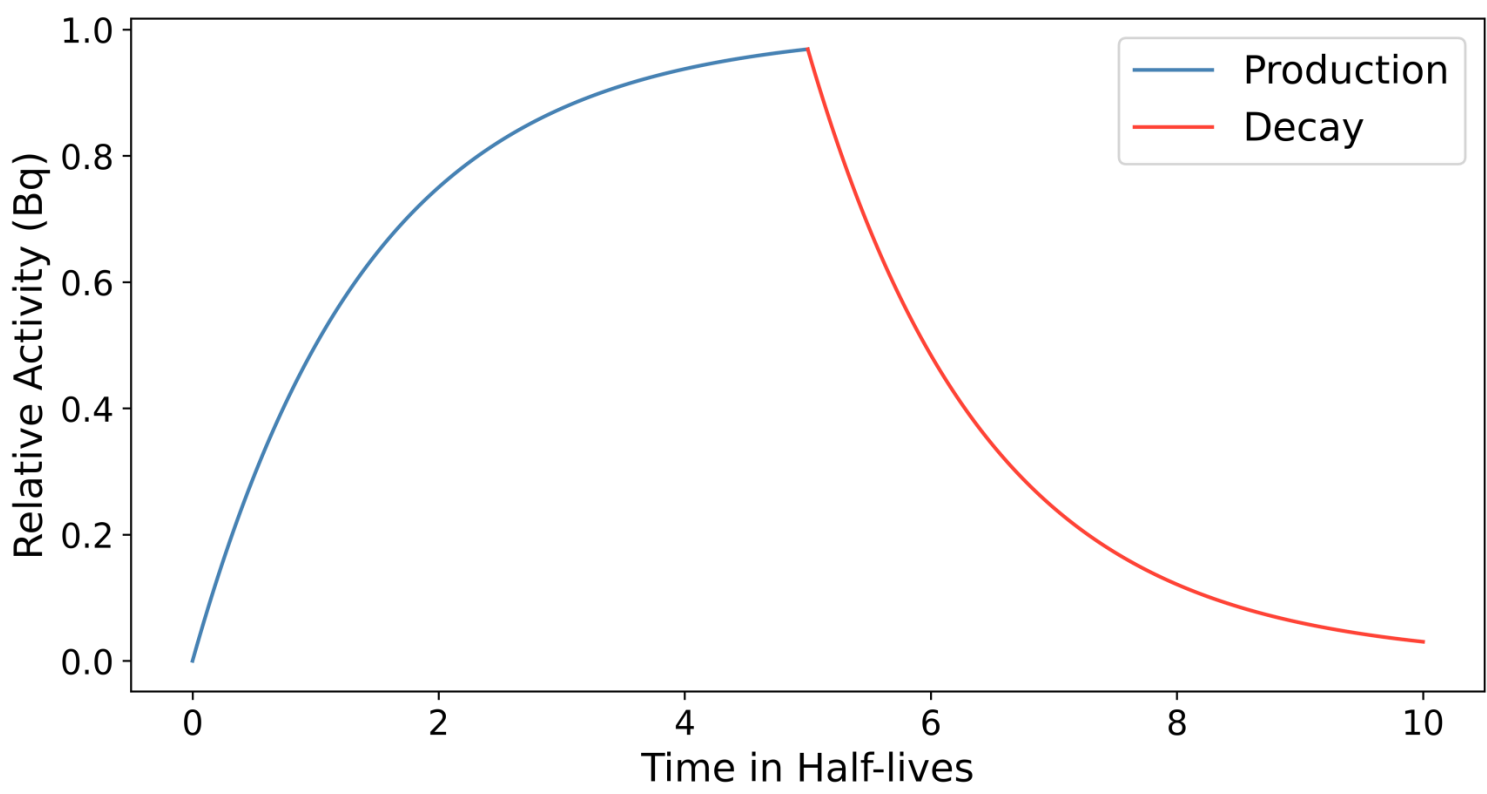


Figure 4) Activity of a sample during and after neutron irradiation.

Activities were calculated at increasing proton energies, resulting in different neutron yields and flux profiles.

Additionally, the effects of increasing thicknesses of graphite moderator were explored.

Plot of simulated Ho-166 activity as a function of proton current.

Plot of simulated Ho-166 activity as a function of moderator thickness.

Conclusion and Outlook

- An OpenMC model has been developed to facilitate activity calculations at HF-ADNeF.
- The rate of a chosen reaction is given by the normalised (n,γ) tally.
- Simulations of different moderator thicknesses show that

Future Work

- Comparison to MCNP, Geant4 and other codes.
- Simulation of neutron spectrum expected in foils, to be fed into other codes to all reaction products.
- Investigation of more complex moderator designs and neutron shaping materials.

Acknowledgements

This work was part funded by the Hawkesworth fund, University of Birmingham. Many thanks to the accelerator staff at HF-ADNeF for the experimental work.

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OpenMC simulations of the UoB HF-ADNeF for Medical Isotope Production

M Conroy¹, T Price¹, M Freer¹, B Slingsby², R Mills²

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Introduction

Each year in the UK, radioisotopes are used in X medical procedures. Currently, production of many of these radioisotopes relies upon the intense neutron fluxes provided by ageing research reactors.

Due to the high cost of building new research reactors, accelerator driven neutron sources may provide an alternative for production of radionuclides on a smaller, local scale. Modern neutron sources, such as the high-flux accelerator driven neutron facility (HF-ADNeF) at the University of Birmingham can produce neutron fluxes of up to $10^{12} \text{ n s}^{-1} \text{ cm}^{-2}$, as seen in Alex's poster.

To investigate the possibility of producing novel isotopes at this facility, an OpenMC simulation has been produced to facilitate calculations of activities that can be achieved given various irradiation conditions.

Model Inputs

Geometry:

A 3D model of the target room has been developed in OpenMC and can be imported as a Python package.

Activation foils, moderating materials and more can be added using functions to prevent boundary clashes.



Figure 1) Side by side comparison between 3D CAD and photograph of target room.

Starting Neutron Information:

A C++ source file is defined based on MCNP input cards, using data from Minsky et al, for each proton energy.

A neutron energy is first sampled via linear interpolation.

Based on this neutron energy, the relevant angular distribution is sampled for the lab emission angle.

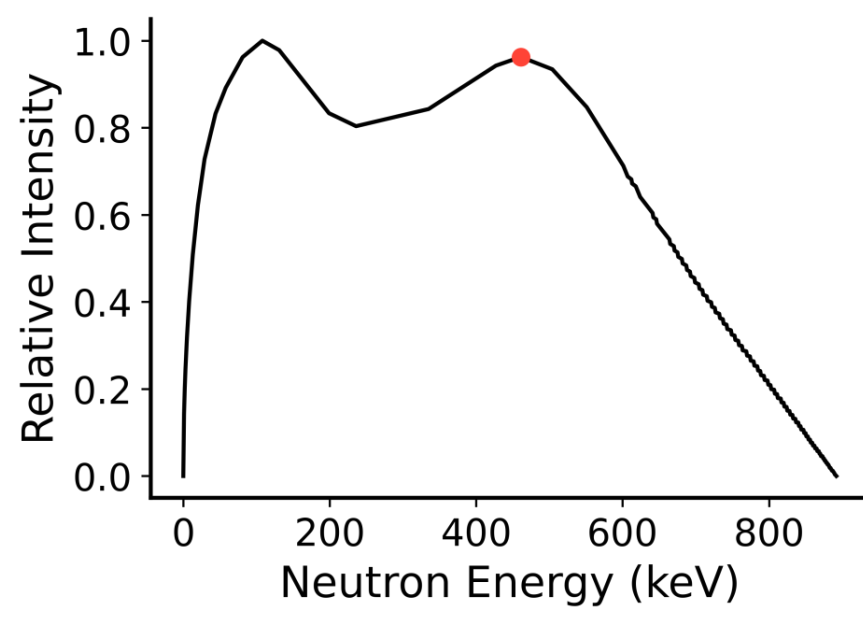


Figure 2) Neutron energy distribution for 2.6 MeV protons incident on target.

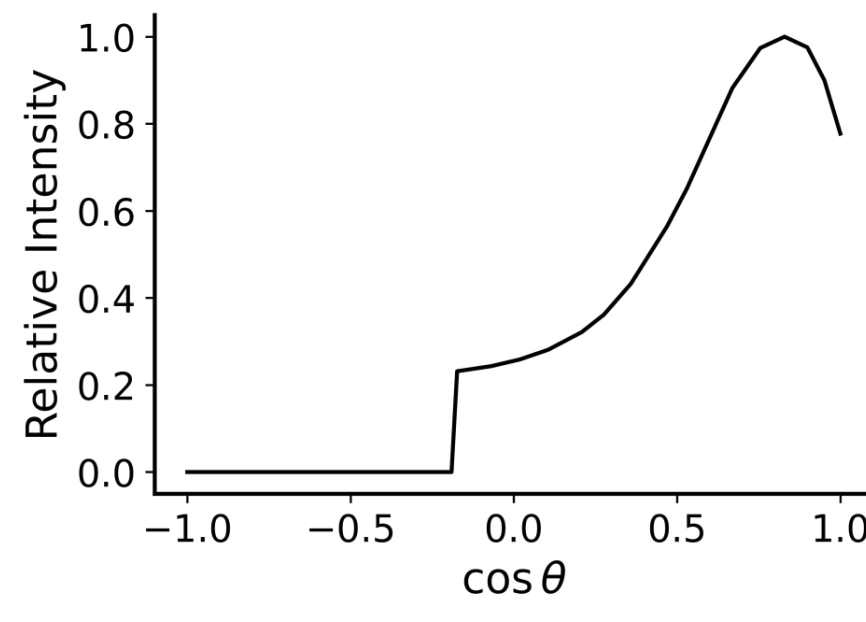


Figure 3) Angular distribution for 461 keV neutron sampled in figure 2.

Model Outputs

Tallies:

For this work, the tallies of interest are **flux** and **(n,y)** in the activation foil.

All tallies are output **per source particle**.

Applying **energy filters** to tallies allow for output neutron energy spectra to be produced.

Result Normalisation:

A **source strength** term gives the number of neutrons per mC of proton beam, also given by Minsky et al.

Multiplying tally results by the strength and proton current gives a **rate**.

The flux tally is given in units n-cm, so must be multiplied by **cell volume** to get units $\text{cm}^{-2} \text{ s}^{-1}$.

Neutron Tracks:

A **track file** contains neutron position and energy information at each step.

This allows for validation and of the **neutron transport** in the problem.

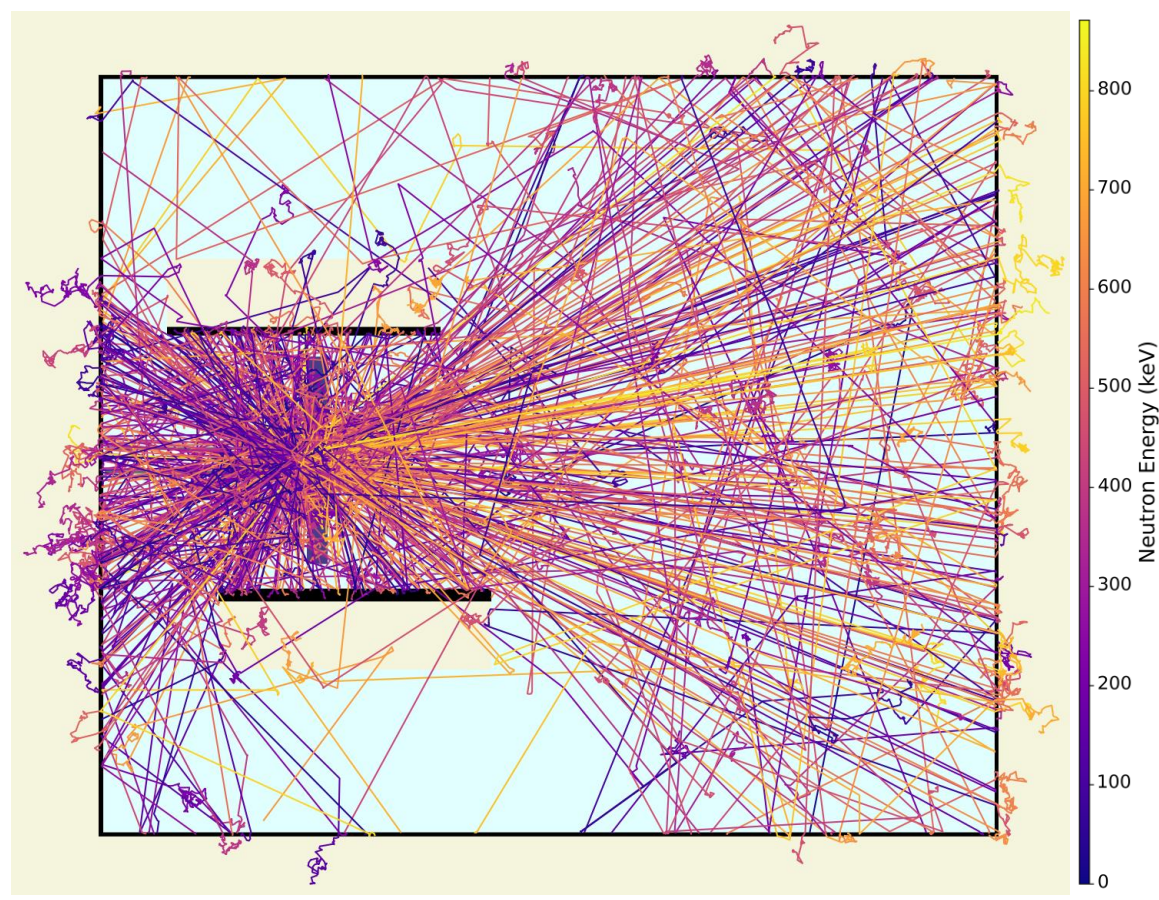


Figure 3) Top-down view of neutron tracks, colour coded by initial neutron energy.

Activity Calculations

The **reaction rate** for producing a given isotope is the **convolution** of the incident flux and the cross section, multiplied by the number density of the target isotope,

$$R = N \int \phi(E) \cdot \sigma(E) dE.$$

The **activity** of a specific isotope at a given time can then be calculated knowing the **half-life** of the product,

$$A = R(1 - e^{-\lambda t_{irr}})e^{-\lambda t}.$$

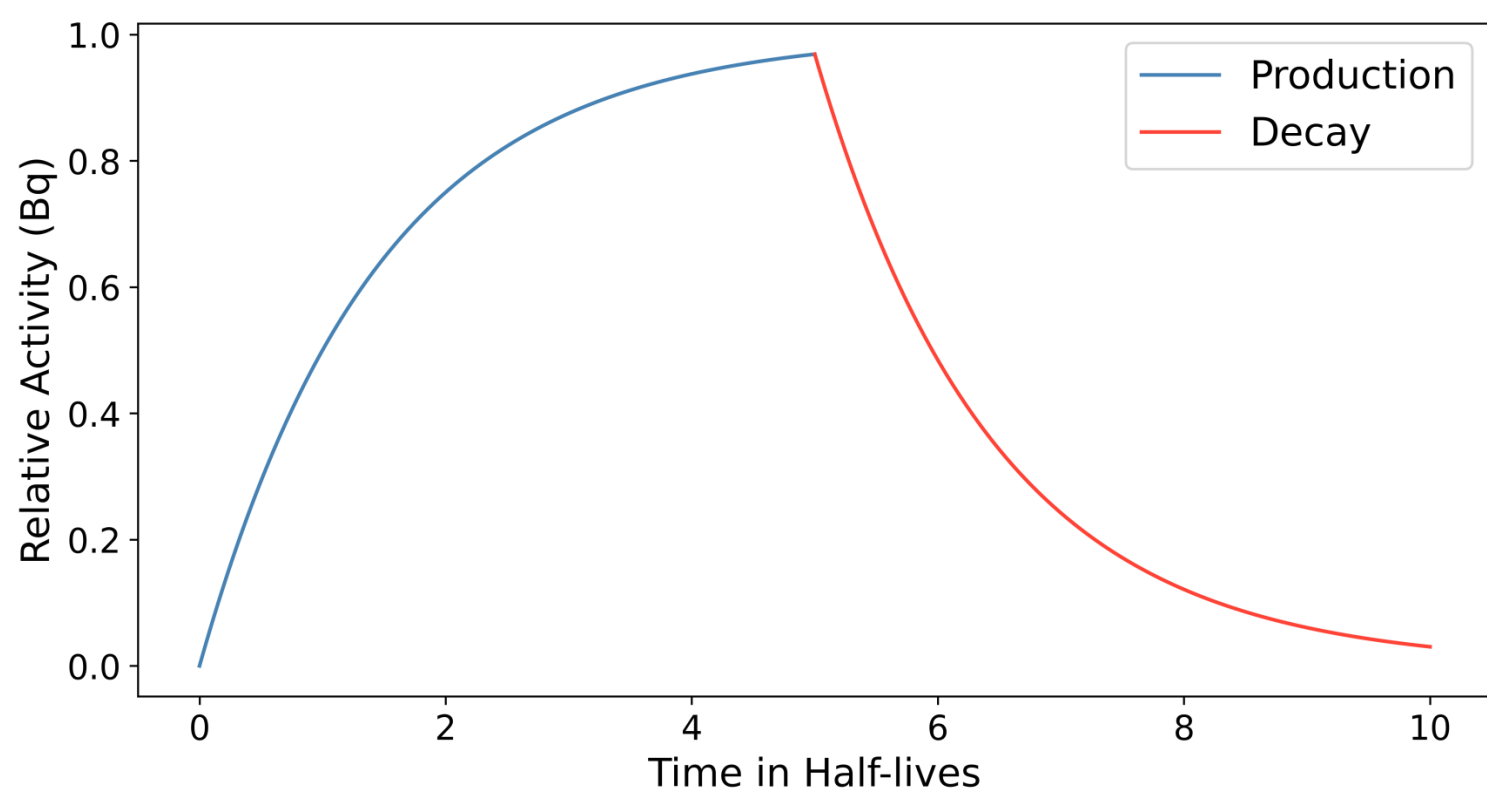


Figure 4) Activity of a sample during and after neutron irradiation.

In this work, the irradiation of a **natural europium** foil was simulated.

Europium has two stable isotopes, ^{151}Eu (47.8%) and ^{153}Eu (52.2%).

The **normalised (n,y)** tallies of each isotope give the reaction rates of ^{152}Eu and ^{154}Eu production.

Since the cross section for neutron capture is 2 orders of magnitude higher for ^{151}Eu than ^{153}Eu , increasing lengths of graphite were introduced to moderate the neutrons.

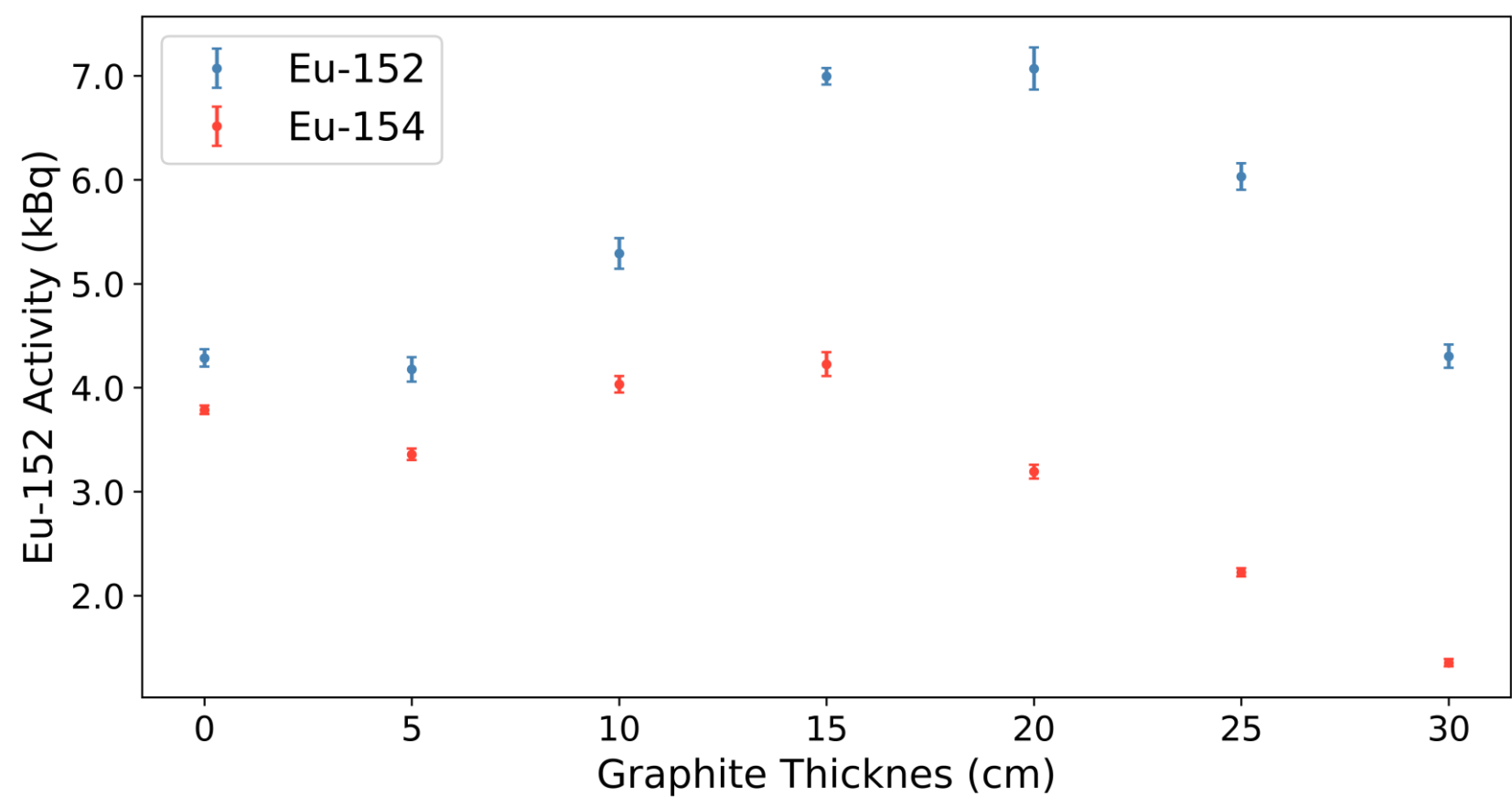


Figure 6) Activities of Eu isotopes in natural foil after 1 hour neutron irradiation, for increasing moderator thickness.

This led to a maximum predicted activity of ^{152}Eu of 7 kBq with 20 cm of graphite, while the ^{154}Eu activity was suppressed.

Experimental Work

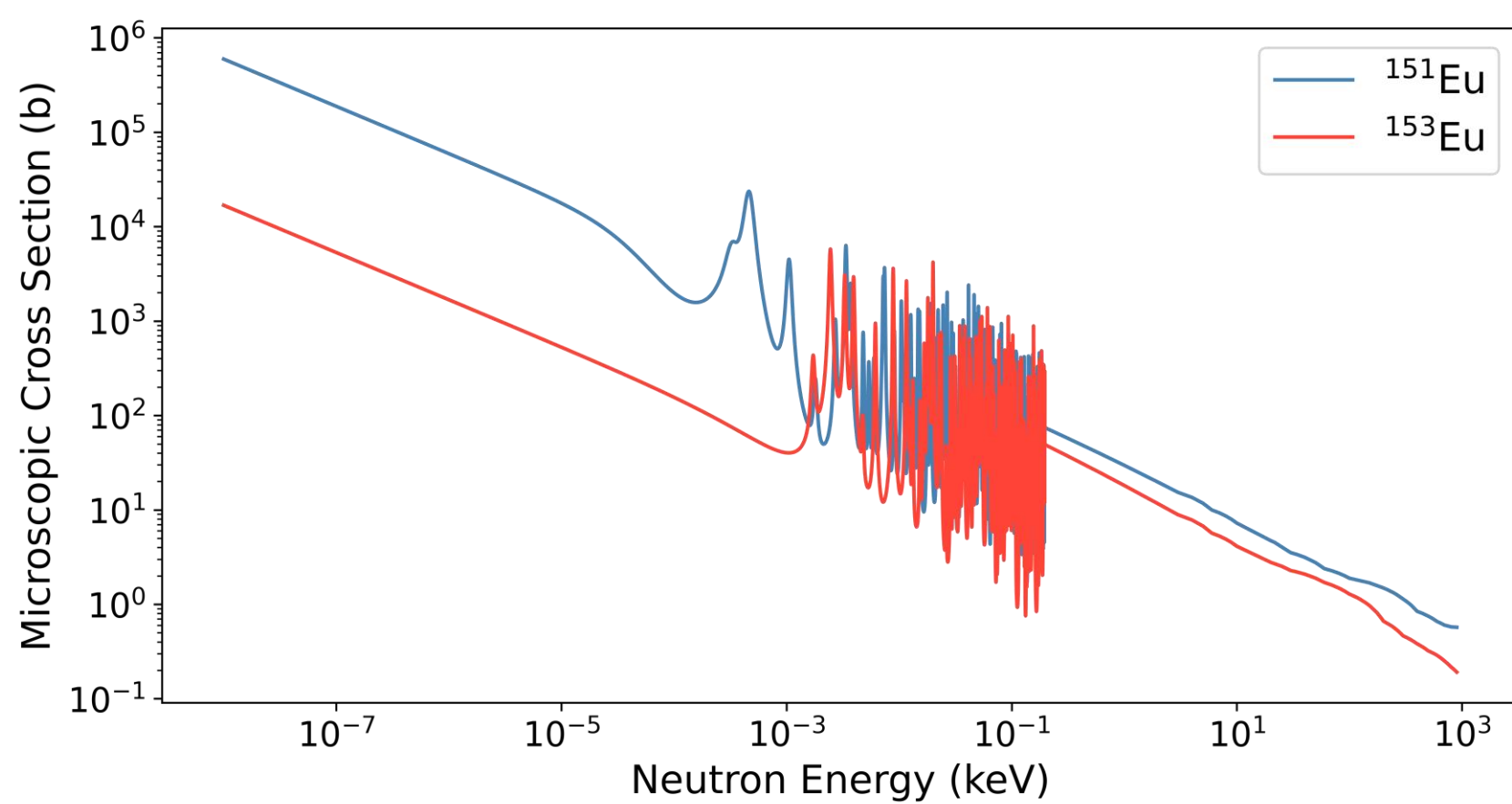


Figure 5) Microscopic (n,y) cross sections of ^{151}Eu and ^{153}Eu in relevant energy range.

Future Work

- Comparison to MCNP, Geant4 and other codes.
- Simulation of neutron spectrum expected in foils, to be fed into other codes to all reaction products.
- Investigation of more complex moderator designs and neutron shaping materials.

Conclusion

- An OpenMC model has been developed to facilitate activity calculations at HF-ADNeF.
- The rate of a chosen reaction is given by the normalised (n,y) tally.
- Simulations of different moderator thicknesses show that

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Introduction

Each year in the UK, radioisotopes are used in X medical procedures. Currently, production of many of these radioisotopes relies upon the intense neutron fluxes provided by ageing research reactors.

Due to the high cost of building new research reactors, accelerator driven neutron sources may provide an alternative for production of radionuclides on a smaller, local scale. Modern neutron sources, such as the high-flux accelerator driven neutron facility (HF-ADNeF) at the University of Birmingham can produce neutron fluxes of up to $10^{12} \text{ n s}^{-1} \text{ cm}^{-2}$, as seen in Alex’s poster.

To investigate the possibility of producing novel isotopes at this facility, an OpenMC simulation has been produced to facilitate calculations of activities that can be achieved given various irradiation conditions.

Model Inputs

Geometry:

- A 3D CAD model of the target and surrounding room has been developed and defined in OpenMC.
- A Python package has been created which allows the geometry to be imported and defined in a single line of code
- Methods in this package allow for additional geometry items, such as activation foils or moderating materials to be added without clashing with the main geometry.



Figure 1) Side by side comparison between 3D CAD and photograph of target room.

Starting Neutron Information:

- Neutrons are produced via the ${}^7\text{Li}(p,n){}^7\text{Be}$ reaction. For a given proton energy, the energy distribution of these neutrons is defined based on MCNP input cards from Dan Minsky.
- A compiled C++ source file is generated for proton energies, where first a neutron energy is sampled from the distribution below, linearly interpolated between points.

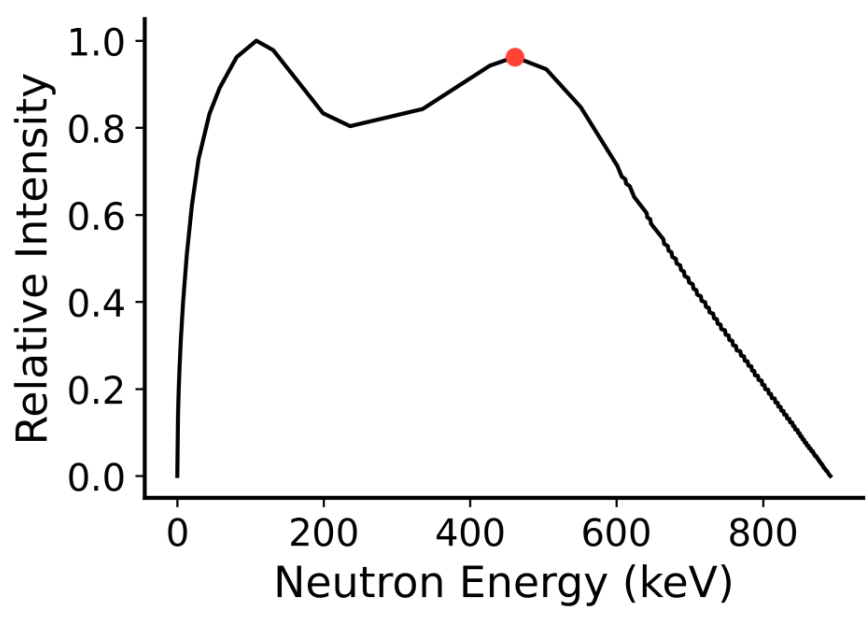


Figure 2) Neutron energy distribution for 2.6 MeV protons incident on target.

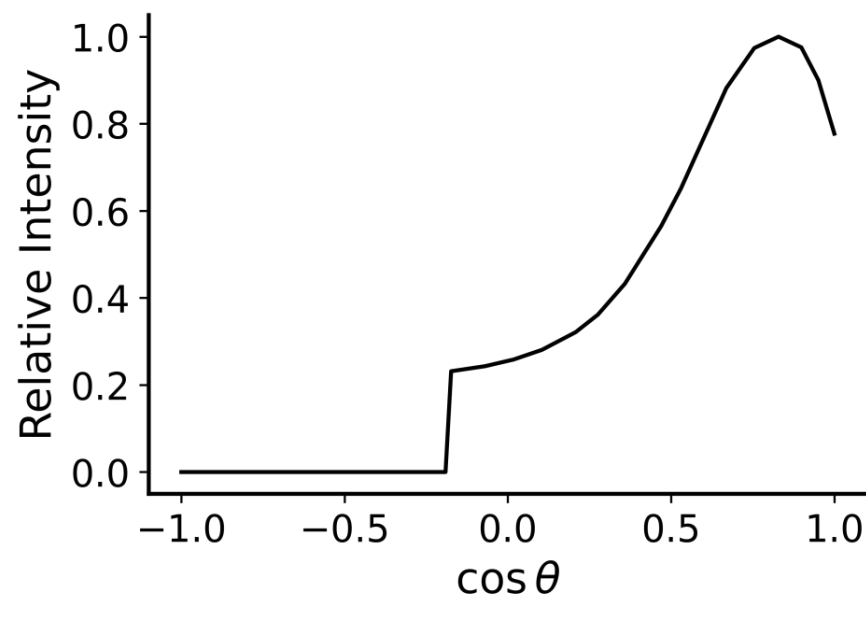


Figure 3) Angular distribution for sampled energy highlighted in figure 2.

Model Outputs

Tallies:

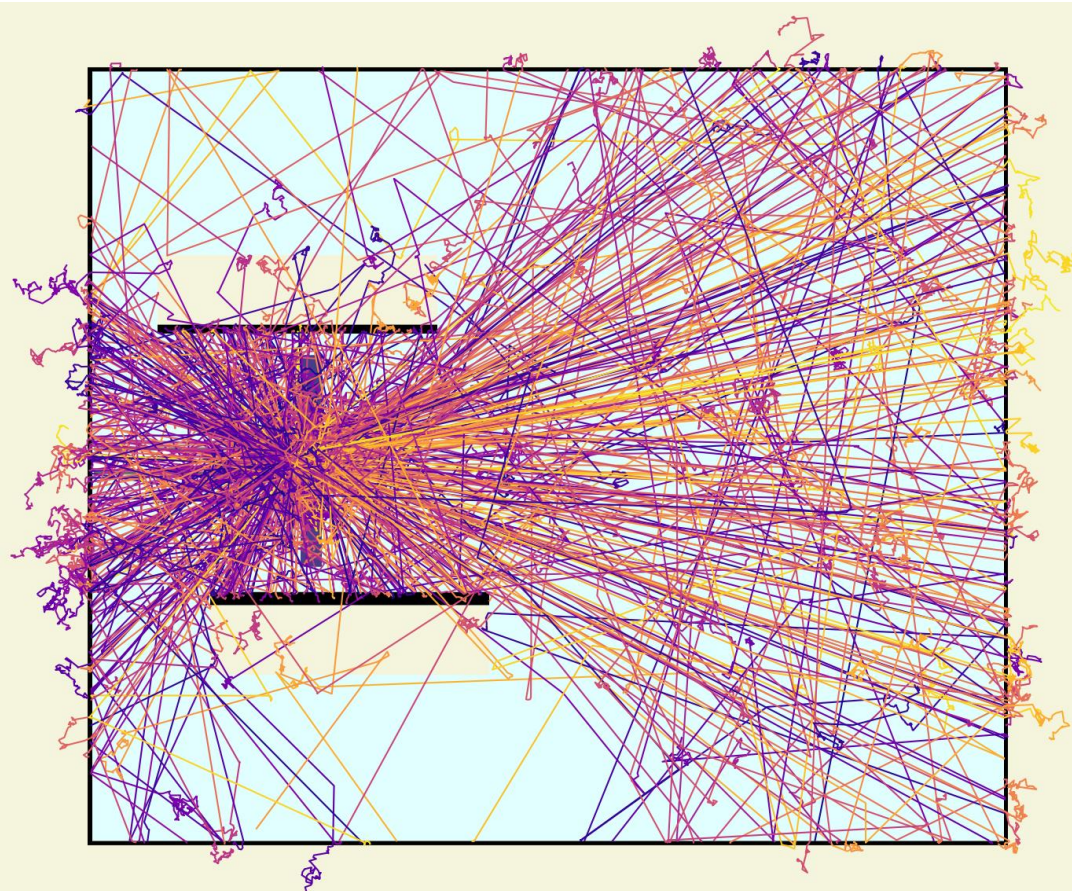
OpenMC supports many tallies. For this work, the most useful are flux and (n,γ) . For detector response, tallies such as (n,α) are useful, for a BF3 detector for example. Applying energy filters to tallies allow for output neutron energy spectra to be produced.

Result Normalisation:

Tallies are output per source particle and for flux, in n-cm. Flux must be normalised by dividing by cell volume. For each incident proton energy, a source strength is defined, giving the number of neutrons per mC of proton beam. Multiplying tally results by the strength and by the proton current (30 mA) gives a flux or reaction rate.

Neutron Tracks:

A track file containing neutron position and energy information at each step can be output. This allows for validation and viewing of neutron transport in problem.



Activity Calculations

Theory

The **reaction rate** for producing a given isotope is the **convolution** of the incident flux and the cross section, multiplied by the number density of the target isotope,

$$R = N \int \phi(E) \cdot \sigma(E) dE.$$

In these simulations, the **normalised (n,γ)** tally gives the reaction rate, **R**.

The **activity** of a specific isotope at a given time can then be calculated knowing the **half-life** of the product,

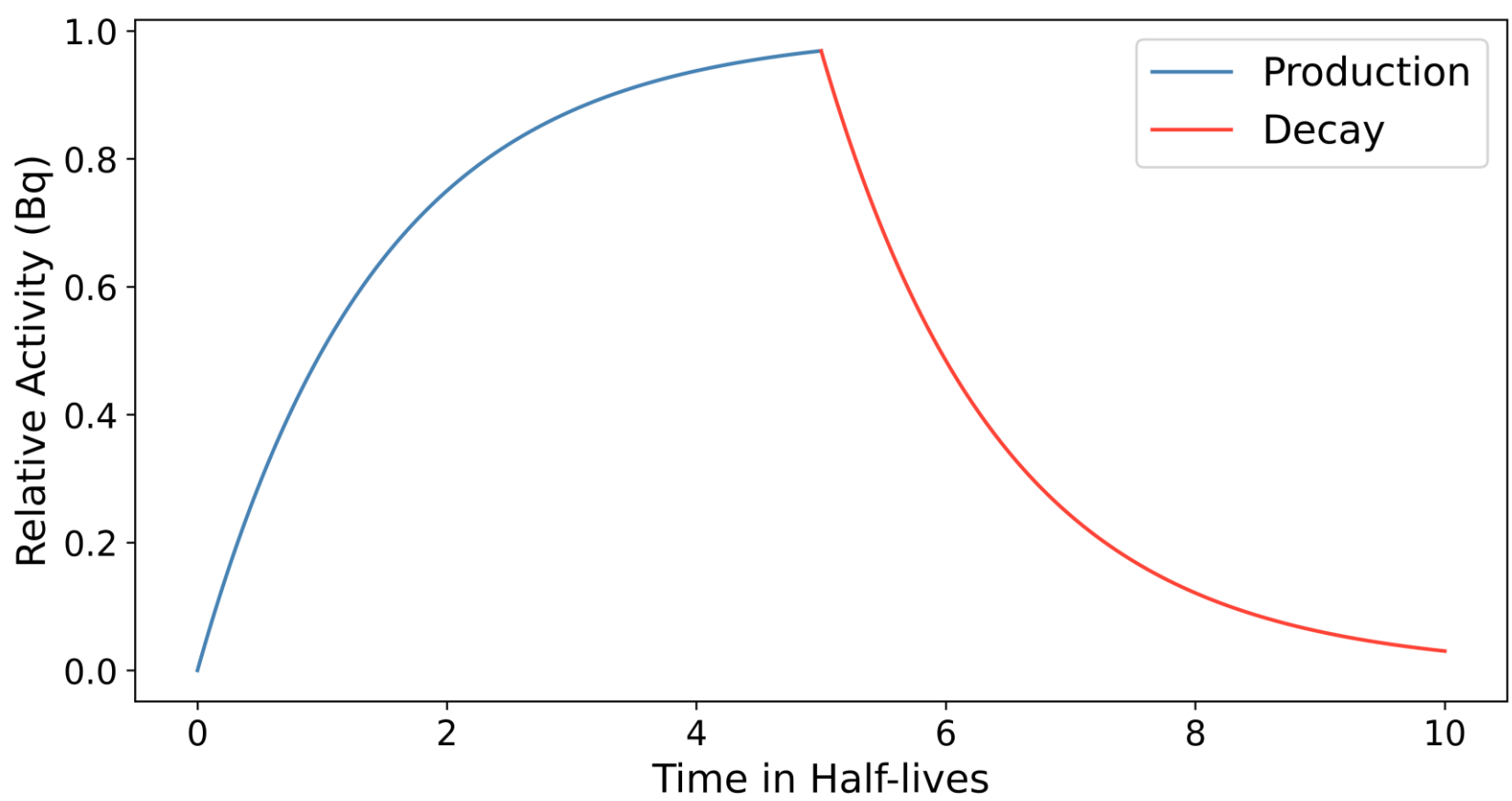
$$A = R(1 - e^{-\lambda t_{irr}})e^{-\lambda t}.$$

Simulation Results

In this work, the irradiation of a natural europium foil was simulated.

The two stable isotopes of europium are ${}^{151}\text{Eu}$ (47.8%) and ${}^{153}\text{Eu}$ (52.2%).

The introduction of a graphite moderator increases the



Experimental Work

Conclusion

Future Work

- Comparison to MCNP, Geant4 and other codes.
- Simulation of neutron spectrum expected in foils, to be fed into other codes to all reaction products.
- Investigation of more complex moderator designs.
- Investigation of neutron shaping materials.
- Full experimental simulations.

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Model Inputs

Geometry:

- A 3D CAD model of the target and surrounding room has been developed and defined in OpenMC.
- A Python package has been created which allows the geometry to be imported and defined in a single line of code
- Methods in this package allow for additional geometry items, such as activation foils or moderating materials to be added without clashing with the main geometry.

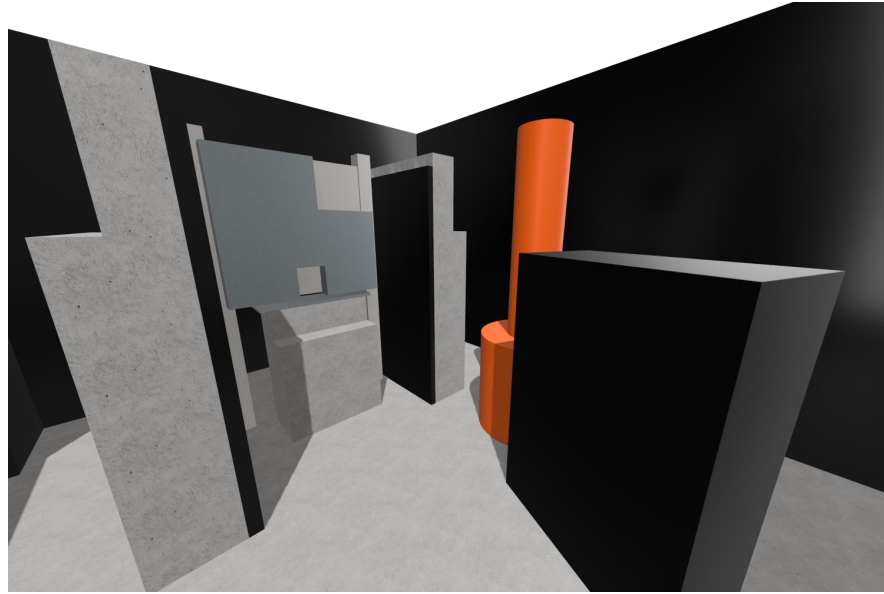
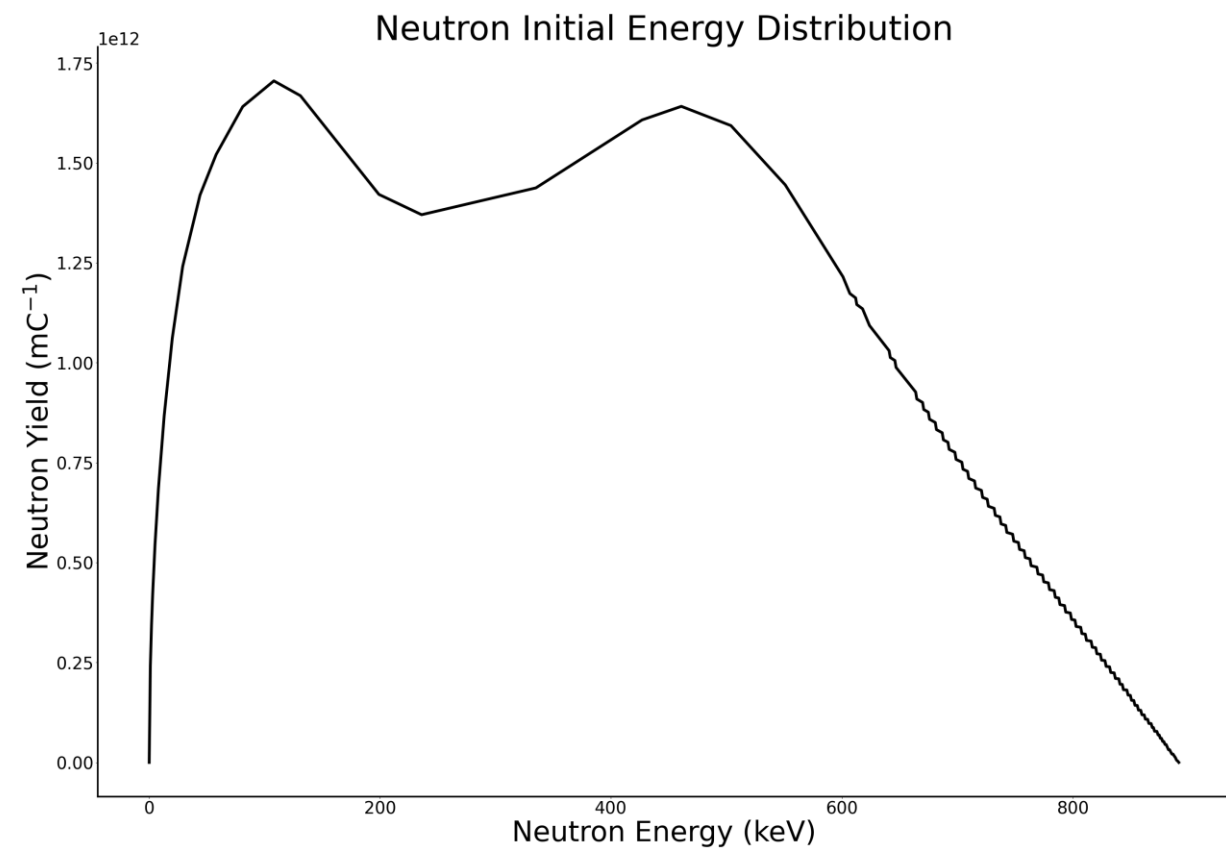


Figure 1) Side by side comparison between 3D CAD and photograph of target room.

Starting Neutron Information:

- Neutrons are produced via the ${}^7\text{Li}(p,n){}^7\text{Be}$ reaction. For a given proton energy, the energy distribution of these neutrons is defined based on MCNP input cards from Dan Minsky.
- A compiled C++ source file is generated for proton energies, where first a neutron energy is sampled from the distribution below.



Activity Calculations

Theory

- For

$$- A = R(1 - e^{-\lambda t - I})$$

Create a plot of activity against time, accounting for production and subsequent decay. Mention saturation after approximately 5 half lives.

Simulation Results

Insert a plot of activity against moderator thickness, formatted nicely.

Can also then discuss a

Experimental Work

Acknowledgements

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