

# Coupling of neutron optics and shielding using Vites and Geant4

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SOURCE

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## Abstract

The European Spallation Source (ESS) will be a material research center built around a powerful neutron source. At ESS, researchers will be able to carry out precise measurements using neutron scattering. The quality of the measurements is determined by the signal-to-noise ratio. The signal consists of neutrons with energies that are useful for experiments, while neutrons with higher energies constitute background noise. Neutron optical systems transport the useful neutrons from the source to the experimental station, and shielding is used to block higher-energy neutrons. Neutrons will also create gamma rays when they interact with matter, and these need to be shielded for safety reasons.

The behavior of the neutron beam is investigated using simulation software. Simulations of neutrons optics and shielding are typically carried out separately, using different types of software. The shielding is studied by simulating the paths of the high-energy neutrons from the source ( $E_k > 1$  eV) using general particle transport software. Lower-energy neutrons are simulated using ray-tracing software that models the neutron optics. The latter do not model scattering of neutrons in the shielding around neutron guides. This could potentially be a problem, since in reality these neutrons might scatter in the guide material and end up as background noise in instruments. If the simulations do not take these neutrons into account, they will not be included in noise estimations. If this noise is not shielded properly it could have a negative effect on instrument performance.

In this project, a method for coupling two software packages for neutron optics and neutron shielding was implemented. The software packages used were the ray-tracing software Vitess and the particle transport software Geant4. A method was added to the source code of Vitess to extract information about neutrons that are not transmitted through neutron optics. This information was passed to Geant4, allowing it to simulate the continued path of these neutrons. The coupling was tested on a simplified neutron guide with different curvatures. The results show that the coupling does have an impact on the background noise coupling effects should be accounted for in signal-to-noise calculations. The coupling will also produce significant amounts of gamma rays, which should be considered when determining radiation levels for safety purposes.

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# Contents

<b>Acknowledgements</b>	<b>iii</b>
<b>1 Introduction</b>	<b>1</b>
1.1 Overview . . . . .	1
1.2 Producing neutrons at ESS . . . . .	3
1.3 Neutron scattering . . . . .	4
<b>2 Neutron physics</b>	<b>6</b>
2.1 Neutron energy . . . . .	6
2.2 Neutron sources . . . . .	7
2.3 Neutron optics . . . . .	9
2.4 Neutron guide geometry . . . . .	10
2.4.1 Guide shape . . . . .	11
2.4.2 Curvature . . . . .	12
2.4.3 Example of a neutron instrument: LoKI . . . . .	13
2.5 Shielding . . . . .	14
<b>3 Signal and noise simulations</b>	<b>17</b>
3.1 Monte Carlo methods . . . . .	17
3.2 Vitess (Virtual Instrumentation Tool for ESS) . . . . .	19
3.3 Geant4 (GEometry ANd Transport) . . . . .	20
3.4 Simulation process . . . . .	22
3.5 Coupling Vitess and Geant4 . . . . .	23
3.6 Geometry of the neutron guide for this project . . . . .	24
3.7 Normalization . . . . .	26
3.7.1 Geant4 output . . . . .	27
3.7.2 Geant4-Vitess coupling output . . . . .	27
<b>4 Results and discussion</b>	<b>29</b>
4.1 Simulation process . . . . .	29

<i>CONTENTS</i>	v
4.2 Signal-to-noise ratio . . . . .	31
4.3 Gamma rays . . . . .	35
<b>5 Conclusion</b>	<b>40</b>
5.1 Outlook . . . . .	40
<b>References</b>	<b>42</b>
<b>Appendices</b>	<b>45</b>
<b>A Translating coordinates</b>	<b>45</b>
<b>B Summary in Swedish</b>	<b>47</b>

# Chapter 1

## Introduction

### 1.1 Overview

The European Spallation Source (ESS) [1] is a research facility that will be located in Lund, Sweden. Planned to start operations in 2019, ESS will be the world's most powerful neutron source. Its purpose is to provide high-resolution neutron beams that will be used to examine materials for a wide range of scientific experiments. A neutron beam acts as precise and non-destructive probe that is able to image structures and movements on small length and time scales, and the uncharged nature of neutrons enables them to travel deep beneath the surface of a sample to reveal its inner structure.

The aim of ESS is to complement existing neutrons sources such as ILL (France) [2], ISIS (United Kingdom) [3], SNS (USA) [4] and J-PARC (Japan) [5]. The focus of ESS will be on condensed matter sciences. Probing condensed matter requires cold and thermal neutrons, in the energy range of 0.1 meV to 50 meV . Most existing neutrons sources are optimized for higher energies, around 100-1000 meV [6]. Another unique feature of ESS is the long pulse duration of the proton beam, 2.86 ms, whereas for example SNS (a short-pulse neutron source) have a proton pulse length on the order of 1  $\mu$ s [7]. The advantage of short-pulse neutron sources is high peak brightness, but long-pulse neutron sources have other merits. The long pulse and low repetition rate (14 Hz) of ESS are ideal for slow, long-wavelength neutrons

in the cold and thermal range. A long pulse also allows for greater flexibility in tailoring the resolution and bandwidth for the neutron instruments.

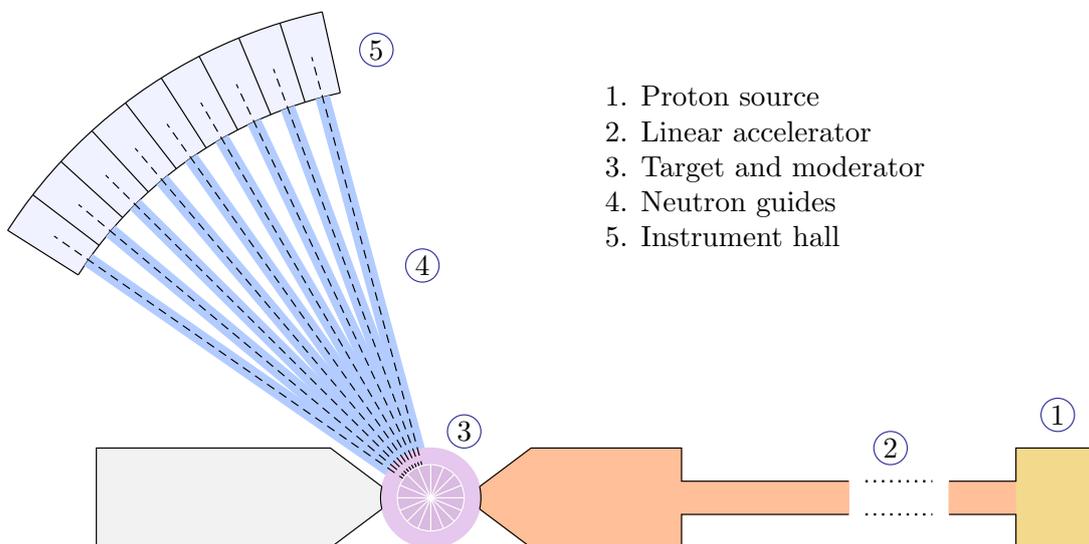
Neutrons created at a spallation source have a wide range of energies. The experiments dictate which energies are interesting. Neutrons of other energies should preferably be filtered out in order to get a good-quality signal. The interesting neutrons are guided towards the sample inside thin guides, taking advantage of the small, yet still present, angle of total reflection. The neutron guides also contribute to a better signal quality. The higher the kinetic energy of the neutrons, the less likely they are to be reflected inside a neutron guide. Because of this, neutron guides are efficient in removing noise in the form of high-energy neutrons.

The reflection process is modeled using special ray tracing software, for example Vitess [8] [9] or McStas [10]. The higher-energy neutrons are modeled using general particle transport software, for example Geant4 [11] or MCNPX [12].

One possible issue with having separate models is that it means ignoring what happens to the low-energy neutrons that fail to reflect all the way through the neutron guide. These neutrons might scatter in the shielding and show up as noise in instruments or at the sample position. This thesis will investigate the contribution of these neutrons to the background noise. In addition, the gamma rays created when these neutrons scatter could potentially be of interest to radiation safety. For this reason, the gamma rays escaping along the guide were also detected.

In this project, Vitess is coupled to Geant4 by adding a function to the Vitess source code that exports information about the neutrons that are lost in the guide. The paths of these neutrons are then simulated using Geant4. Similar work has been done by coupling McStas and MCNPX [13], as well as Vitess and MCNPX [14]. The reason that this thesis focuses on Vitess and Geant4 is that these software packages are commonly used at ESS, and there is no pre-existing coupling of the two. An argument for using Geant4 is that it is open-source and can be modified. Geant4 also has a large user base, since it is used in the high-energy physics community.

## 1.2 Producing neutrons at ESS



**Figure 1.1:** Schematic picture of ESS.

The main components of ESS are shown in Figure 1.1. Below is a brief description of each part [6].

*Proton source.* (1) Protons are produced by heating hydrogen until it forms a plasma of free electrons and protons. The protons are separated from the electrons by an electric field. Protons are released into the accelerator in pulses of 2.86 ms.

*Linear accelerator.* (2) The protons are accelerated to 2 GeV, which corresponds to 96% of the speed of light, in a linear accelerator.

*Target.* (3) Neutrons are emitted when the protons collide with the atoms of the target material. The target material is tungsten (W) in the form of slabs mounted on a rotating wheel. In order to avoid overheating, a new section of target material is exposed for each beam pulse, and the wheel is cooled using a helium gas system. Each incoming proton will generate about 80 neutrons.

*Moderator.* (4) Two different moderating materials slow down the neutrons to thermal and cold levels, respectively. The thermal source is room-tempered water and the cold source is super-critical hydrogen at a temperature of 13-20 K.

*Instruments.* (4) (5) The instrument system includes neutron guides, as well as beam modifying instruments that are placed along or the end of guides. Instruments can be used to reduce beam divergence, filter out neutrons with unwanted energies, or to perform measurements on the beam. One important device is the neutron beam chopper. A chopper consists of a rotating disc that is tuned to let through neutrons of a specific wavelength range.

*Neutron guides.* (4) Neutron guides are part of the instrument system. Guides steer the neutrons from the source to the sample position. The guides can be coupled to the cold source or the thermal source, or a combination of both.

*Sample environment.* (5) The neutron beam is focused on a material sample. The conditions of the sample environment will vary greatly depending on the experiment. The electric field, magnetic field, temperature, pressure and humidity need to be controlled precisely and over a wide range. Temperatures can range from a few mK to thousands of K, magnetic fields from 0 to 17 T.

*Detector.* (5) The neutrons are either scattered on the sample or transmitted through it. They are then absorbed in detectors that surrounds the sample. Because neutrons have no charge, they cannot be detected electronically themselves. They must first interact with a material in a way that creates charged secondary particles.

### 1.3 Neutron scattering

Neutron scattering is used to study atomic-scale structures of materials. The sample is placed in the neutron beam and the neutrons that are scattered or transmitted are detected. Periodic structures in the material give rise to interference patterns in the detected neutrons. This is similar to how x-ray scattering and electron microscopy work. Some advantages of using neutrons for measurements are [6]:

- Thermal neutrons have wavelengths on the same order of magnitude as interatomic distances in condensed matter, making them useful for investigating atomic structures.

- Thermal neutrons also have energies of the same scale as inner movements in solid and liquids. This makes it possible to measure fluctuations inside materials using neutrons.
- Neutrons will travel further beneath the surface than photons or electrons, allowing them to probe structures deep inside materials. Neutrons interact with matter through the strong nuclear force. This force has a very small interaction radius, only a few femtometers. As a result, neutrons view solid materials as sparse compared to electrons and photons that interact with the atomic electrons.
- The interaction probability of neutrons to an atom depends on the atom's nuclear composition and is usually very different than for electrons and photons. Neutrons are most sensitive to hydrogen. Neutrons can distinguish between isotopes and see light atoms in the presence of heavy atoms. For example, neutrons can image structures of plastic or wood underneath a metal coating. This makes neutron scattering a good complement to x-ray scattering, for which the sensitivity increases with atomic number.
- The uncharged nature of neutrons makes them non-destructive. Neutrons can be used to investigate rare and fragile objects, such as valuable artwork and historical artifacts.
- Neutrons have a magnetic dipole moment. This allows them to measure atomic-level magnetic structures.

# Chapter 2

## Neutron physics

This chapter introduces the physics necessary to understand neutron guides and neutron shielding. The discussed concepts are neutron energy, neutron sources, neutron optics and how it can be applied to design neutron guides, and lastly neutron and gamma ray shielding.

### 2.1 Neutron energy

The kinetic energy  $E_k$  of a neutron is related to its wavelength according to the de Broglie formula

$$E_k = \frac{h^2}{2m\lambda^2}, \quad (2.1)$$

where  $\lambda$  is the de Broglie wavelength of the neutron,  $m$  is the neutron mass and  $h$  is Planck's constant. With energy given in meV and the wavelength in Å ( $10^{-10}$  m), this formula can be approximated with

$$E_k [\text{meV}] \approx \frac{81.81}{\lambda^2 [\text{Å}]}. \quad (2.2)$$

Because neutrons are uncharged it is not possible to accelerate them to higher energies the way protons and electrons are in accelerators, using electric fields. However, neutrons can be slowed down by allowing them to collide with atoms of a moderating medium, thereby transmitting some of their kinetic energy to their surroundings, until they reach a state of equilibrium. The temperature of the moderator decides the final speed of the neutrons - the colder the material, the slower the neutrons. Using a room-temperature moderating medium will result in *thermal neutrons* that have a kinetic energy of about 25 meV. A common moderator is regular water, due to the large cross-section for neutron scattering of hydrogen. Hydrogen nuclei are similar in mass to neutrons, which allows for efficient energy transfer.

Neutrons with energies between 50  $\mu\text{eV}$  and 25 meV are called *cold neutrons*. Cold and thermal neutrons are both categorized as slow neutrons. The categorization of neutron energies differs depending on the applications but the categories used in this thesis are the ones in Table 2.1

	Energy	Wavelength
Slow neutrons	$E < 1 \text{ eV}$	$\lambda > 0.3 \text{ \AA}$
Intermediate neutrons	$E = 1 \text{ eV} - 1 \text{ MeV}$	$\lambda = 3 \cdot 10^{-4} \text{ \AA} - 0.3 \text{ \AA}$
High-energy neutrons	$E > 1 \text{ MeV}$	$\lambda < 3 \cdot 10^{-4} \text{ \AA}$

**Table 2.1:** Classification of neutron energies.

## 2.2 Neutron sources

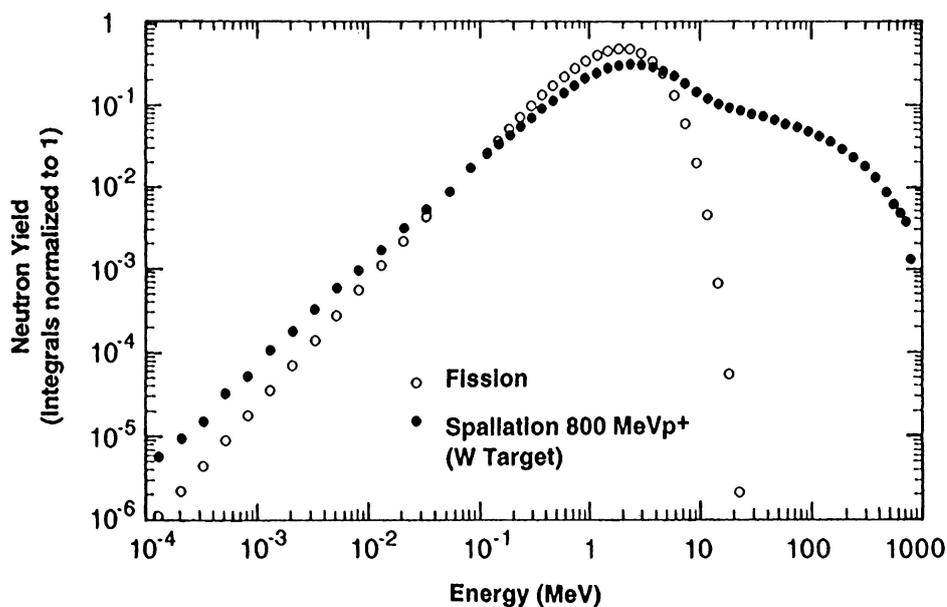
The two main techniques for producing large quantities of neutrons are nuclear fission and nuclear spallation.

Fission is the process of splitting a uranium or plutonium nucleus into lighter nuclear fragments. It is mainly used to generate energy in power plants. Heavy atoms have a higher neutron-to-proton ratio than lighter atoms. Therefore, when heavy atoms are split the reaction releases free neutrons. Fission is a self-sustaining process since the emitted neutrons will continue to split the heavy nuclei in a chain reaction.

Nuclear spallation occurs when a high-energy particle collides with a heavy atomic nucleus, causing it to emit a large number of particles, including

neutrons. Spallation happens in two stages. At the initial collision, the target nucleus ejects high-energy particles that will be absorbed by other nuclei. The second stage is when all the target nuclei are de-excited by emitting many low-energy particles. Neutrons are emitted during both stages, and the neutrons coming from a spallation source can therefore have both very high and very low energies. The highest-energy neutrons that are emitted during the initial collision can be almost as high in energy as the incident projectile particle.

Spallation facilities use protons, accelerated to around 1 GeV in particle accelerators, as projectile particles. Common target materials are tungsten and mercury. Spallation is not a self-sustaining process. Spallation is an endothermal reaction and it cannot be used to generate energy. An influx of high-energy protons is needed to keep the nuclear spallation going.



**Figure 2.1:** Calculated neutron spectra for fission and spallation. [15]

Figure 2.1<sup>1</sup> shows two typical energy spectra of neutrons created by spallation and by fission. Spallation creates neutrons of a wider range of energies than fission. This puts higher demands on shielding, in order to protect instruments from high-energy neutrons.

<sup>1</sup>Reprinted from Nuclear instruments and methods in physics research, 463(3):505-543, G.S. Bauer, Physics and technology of spallation neutron sources, 39., 2001, with permission from Elsevier.

## 2.3 Neutron optics

Because of their wave-like nature, neutrons exhibit behavior usually associated with light, such as interference and reflectance. Neutron transport through a particular material is described by the neutron refractive index  $n$  [16], as given by

$$n^2 = 1 - \lambda^2 \frac{Nb}{2\pi}, \quad (2.3)$$

where  $N$  is the atomic density and  $b$  the coherent scattering amplitude. Because the refractive index is less than 1 for most materials, neutrons will be totally reflected if their inclination angle is smaller than a critical angle  $\theta_c$ , given by

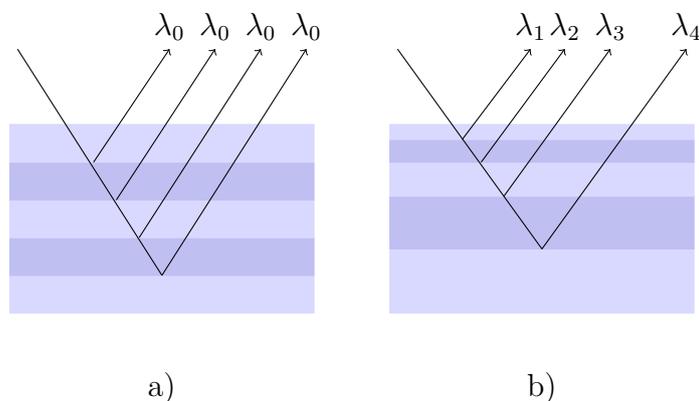
$$\theta_c = \arcsin\left(\lambda \sqrt{\frac{Nb}{\pi}}\right). \quad (2.4)$$

Given a small enough inclination angle, neutrons will travel through a tube by multiple reflections without being absorbed by the walls. This has an added advantage of filtering out high-energy neutrons that have short wavelengths and therefore a small total reflection angle.

The total reflection angle is usually very small, less than a milli-radian (mrad) for most materials. It can be increased by coating the guide with a more reflective material. The most reflective natural material for neutrons is nickel, with a total reflection angle of 1.7 mrad for  $\lambda = 1 \text{ \AA}$ . Higher reflectance can be achieved by taking advantage of wave interference. A so-called Bragg mirror is created by layering materials of high reflective index between materials of low refractive index. A Bragg mirror can be described by the Bragg equation

$$m\lambda = 2d \sin \theta, \quad (2.5)$$

where  $d$  is the layer thickness and  $m$  is a positive integer. If a beam with wavelength  $\lambda$  and incident angle  $\theta$  satisfies the Bragg equation the reflected



**Figure 2.2:** a) Bragg mirror, b) Supermirror

parts of the beam will interfere constructively which leads to high reflection (Figure 2.2a).

By increasing the layer thickness just slightly for each layer, it is possible to get high reflectivity for a range of wavelengths and angles. This is called a *supermirror* (Figure 2.2b).

Supermirrors are characterized by their *m-value*. The standard material for neutron guides is natural nickel, which is given the m-value 1. A supermirror with a total reflection angle twice that of nickel has  $m=2$ . It is possible to manufacture supermirrors with m-values as high as 7.

## 2.4 Neutron guide geometry

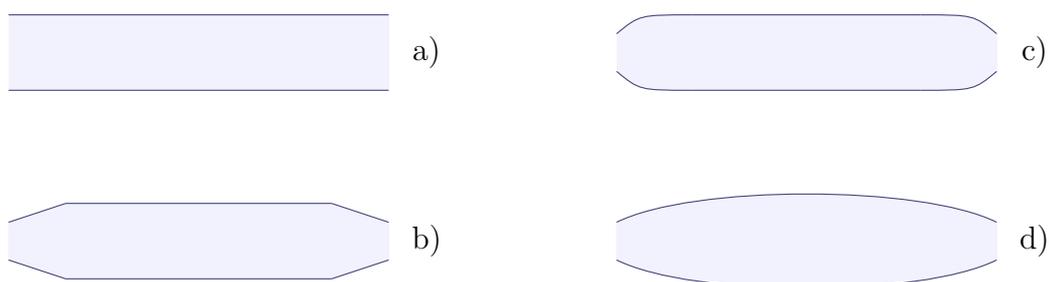
Neutron guides make it possible to conduct experiments with the neutron beam at far distances from the neutron source. Figure 2.3 shows sample pieces of neutron guides made from different materials. The inside of the guides are coated with supermirror material.



**Figure 2.3:** Sample pieces of neutron guides. Left: Close-up of a glass neutron guide. Right: Neutrons guides made of aluminum, glass and copper.

### 2.4.1 Guide shape

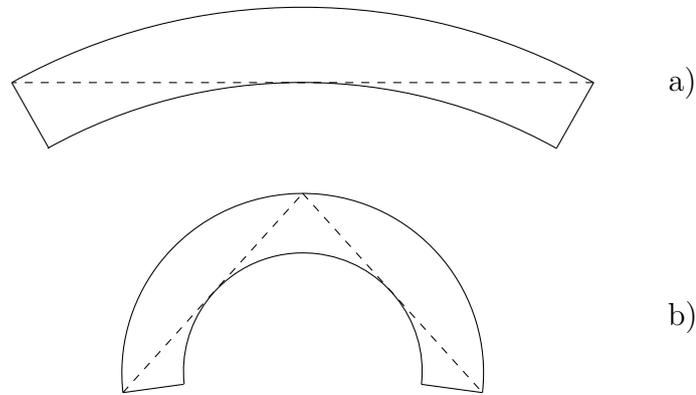
Because the signal is attenuated with each reflection it would be preferable to minimize the amount of reflections by making the neutron beam less divergent. This can be done by replacing the straight guide with a so-called ballistic guide, as seen in Figure 2.4. The simplest way to create a ballistic guide is with linear tapering at each end (Figure 2.4b). A more advanced option is an elliptic guide (Figure 2.4d). A ballistic guide with parabolic tapering (Figure 2.4c) is a less expensive alternative to a fully elliptic guide [17].



**Figure 2.4:** a) Straight guide; b) Ballistic guide with linear tapering; c) Ballistic guide with parabolic tapering; d) Elliptic guide.

## 2.4.2 Curvature

Using curved neutron guides can improve the signal-to-noise ratio. Figures 2.5a-b show a guide section with increasing curvature (the width of the guide is exaggerated to show the curvature better - a realistic beam guide is narrow and very long, and the curvature is barely noticeable). A *line-of-sight* guide has exactly one straight path through the guide (Figure 2.5a). Two line-of-sight sections put together create a guide that is twice the line-of-sight (Figure 2.5b).



**Figure 2.5:** a) Line-of-sight guide. b) 2 times line-of-sight guide.

A guide of length  $L$  and width  $a$  that is  $k$  times out of line-of-sight will have the radius of curvature

$$R = \frac{L^2}{8ak^2}. \quad (2.6)$$

Real guides can be either truly curved or composed of straight pieces put together at an angle. The latter is easier to manufacture, and for long neutron guides the difference between these two designs becomes negligible.

A guide that is curved out of line-of-sight ensures that no particles will be transmitted without interacting with the walls. A MeV neutron that collides with the walls will give rise to a particle shower, with particles of different

energies emitted in all directions. Some of these will be high-energy particles emitted in the direction of the guide. This is why a guide that is just out of line-of-sight might not be enough to block high-energy particles. ESS recommends that neutron guides are at least two times out of line-of-sight. In a curved guide there will also be loss of useful, low-energy neutrons. Choosing the optimal guide length and curvature is a trade-off between suppressing noise and getting high signal.

The supermirror coating should be optimized for the guide curvature. A useful formula for choosing a good  $m$ -value for the coating is

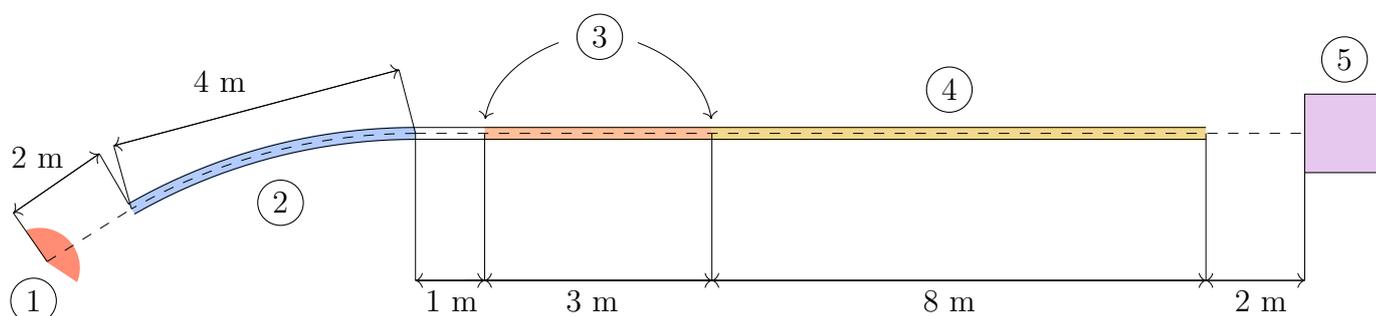
$$m = \frac{1}{\lambda^* \cdot 0.0017} \sqrt{\frac{2a}{R}}. \quad (2.7)$$

Here,  $a$  is the width of the guide,  $R$  is the radius of curvature and  $\lambda^*$  is the *characteristic wavelength*, or the cut-off wavelength for the guide. What this actually means is that no more than 2/3 of the intensity will be transmitted for wavelengths shorter than  $\lambda^*$  [18]. One way to lower the optimal  $m$ -value of a guide is to divide the guide lengthwise into channels with walls in-between. This reduces the effective guide width  $a$ . The radius of curvature is kept the same. Because the thickness of the walls is only 0.5 mm, there will be little interaction between high-energy neutrons and the walls.

### 2.4.3 Example of a neutron instrument: LoKI

LoKI is one of the neutron instruments that will be used at ESS. It will be used for small-angle neutron scattering (SANS) experiments and will focus on biophysics and soft matter studies.

Figure 2.6 shows a layout of the LoKI instrument from the LoKI proposal [19]. The instrument will be coupled to the cold moderator (1). The first part of the guide consists of a curved guide section (2) that ensures that the source is 2 times out of line of sight at the sample position. The curved section is split into 4 channels with  $m=4$  supermirror coatings. Wavelength selection is carried out by two beam choppers (3), placed 3 m apart. The function of the second chopper is to prevent frame overlapping, which happens when



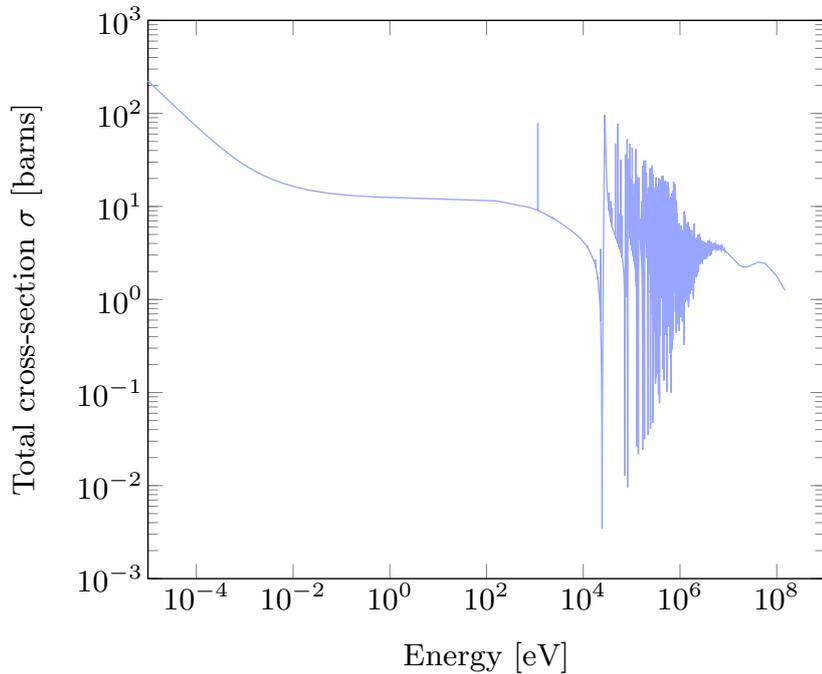
**Figure 2.6:** The LoKI neutron instrument.

slow neutrons from one pulse get overlapped by fast neutrons from the next pulse. The remaining section of the neutron guide (4) contains apertures that collimate the neutron beam. The sample area (5) is surrounded by a 10 m tube lined with detectors.

## 2.5 Shielding

Radiation in the form of high-energy neutrons and gamma rays must be shielded, both for safety reasons and to reduce background noise in instruments. The *cross-section*  $\sigma$  is the probability of interaction between a neutron and the surrounding material. The shielding material must have a high cross-section for the neutrons that are transmitted. The interaction between neutrons and atomic nuclei depends strongly on the neutron energy and the composition of the nucleus. An example of a cross section spectrum (iron,  $^{56}\text{Fe}$ ) is seen in Figure 2.7.

Two types of neutron reactions can occur: direct reactions and compound nucleus reactions [21]. A direct reactions is when the neutron is deflected by a nuclear potential. In a compound reaction, the neutron is first captured by the nucleus to form a short-lived compound nucleus. The compound nucleus decays by emitting a neutron. The reaction is called *elastic* if the energy of the emitted neutron is the same as the energy of the incident neutron, otherwise the reaction is *inelastic*. Compound reactions can only occur if the sum of the neutron's kinetic energy and the neutron binding energy correspond to a quantum energy state of the nucleus. The compound reaction can be seen in the spectrum in the rapidly varying region. The peaks



**Figure 2.7:** Neutron cross-section for  $^{56}\text{Fe}$ . [20]

and valleys are due to constructive or destructive interference.

The slowly varying cross-section in the rest of the spectrum is due to direct reactions. At low energies, the energy dependence of the cross-section is  $\sigma \sim 1/\sqrt{E}$ , which corresponds to the initial downward slope in the spectrum. In this energy region, neutrons will not interact with the individual nuclei but with the vibrational modes (phonons) in the structure of bound nuclei as a whole. In the near-constant region in the spectrum, the energy is still too low to form a compound nucleus. The incident neutron sees each nucleus as a potential. The cross-section is proportional to the area of the nucleus. At high energies, the cross-section drops off [22].

It is important to consider the cross-section when choosing the shielding material. This means that different shielding materials might be used for different sections of the guide, depending on how the energy spectrum of the neutrons and gamma radiation look at that particular place. It can also be beneficial to layer different materials in a way so that resonance peaks and valleys cancel each other out.

Common shielding materials are concrete, plastic and steel. Concrete contains hydrogen, which is effective in moderating high-energy neutrons. Concrete is an inexpensive material that can be used to make thick walls for shielding that will also stop gamma rays. Plastic will slow fast neutrons ( $E_k < 20$  MeV). Steel is a dense material that slows down fast and high-energy neutrons. Some types of steel are not suitable for neutron shielding. Mild steels have energy regions of transparency for neutrons and stainless steel is easily activated by neutron capture. Thermal and cold neutrons can be stopped by materials that contain boron, for example plastics made with boric acid [17].

## Chapter 3

# Signal and noise simulations

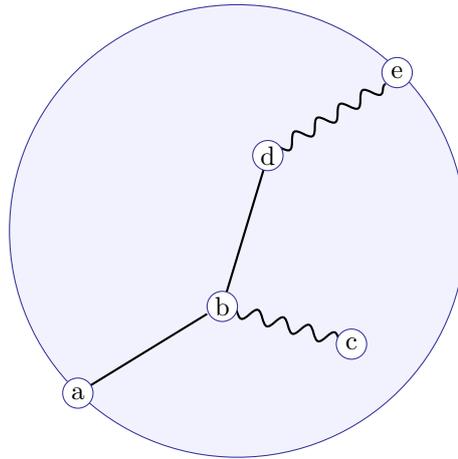
This chapter explains how neutron optics and shielding are simulated using Geant4 and Vitess. Sections 3.1 - 3.4 describe the software packages Geant4 and Vitess and how they are used. Sections 3.5 - 3.7 outlines the process of coupling Vitess and Geant4, and describes the example geometry used to test the coupling.

### 3.1 Monte Carlo methods

Both Geant4 and Vitess use Monte Carlo methods to simulate the paths of particles. Monte Carlo methods are useful for complex problems with many parameters. Rather than making precise predictions, they rely on probabilities to generate possible outcomes that are used to approximate a solution to the problem. The approximation gets better when the number of generated outcomes increase.

An example of a simulated neutron path is shown in Figure 3.1. A path starts with an incident particle entering the defined geometry and ends with the particle being absorbed or leaving the geometry. The simulation software

moves the particle one step at a time. At each step, the particle has a probability of undergoing an event. For example, a neutron that collides with an atomic nucleus might be scattered, absorbed, or splitting the nucleus by fission. Whether an event will occur is decided by sampling a random number from a probability distribution. If a secondary particle is created during the event (for example, a gamma particle), the path of the secondary particle is also tracked.



**Figure 3.1:** a) Incident neutron; b) Neutron scattering and gamma particle emission; c) Gamma particle absorption; d) Neutron absorption and gamma particle emission; e) Gamma particle escapes.

In this project, Geant4 and Vitess were used to approximate how a neutron beam (containing  $\sim 10^{15}$  neutrons per second) behaves in a neutron guide. A path is generated for a number of incident neutrons ( $10^6 - 10^9$  neutrons, depending on the simulation). After simulating a large number of paths, the total collection of outcomes provides a good approximation of how a neutron beam would behave in a guide. An important distinction between Geant4 and Vitess is that Geant4 is a general particle transport program while Vitess is specific to neutrons. Vitess does not simulate secondary particles like gamma rays and electrons.

## 3.2 Vitess (Virtual Instrumentation Tool for ESS)

Vitess is an open-source software package used to simulate neutron scattering. As the name suggests, Vitess was created for ESS, but it can be used for any neutron source. It allows the user to simulate a neutron scattering instrument by placing modules representing different parts, such as neutron sources, guides and detectors. Each type of module is represented by a separate file in the source code.

Neutron guides are modeled using the modules *guide*, that describes an approximated curved guide composed of several straight pieces put together at an angle, or *bender*, that describes a curved guide without kinks. Real neutron guides can be constructed in both ways. The parameters that can be specified for both modules are:

- Width, height and length.
- m-value of the wall coating (as described in Section 2.3).
- Radius of curvature (as described in Section 2.4.2).
- Number of channels (as described in Section 2.4.2))

The multi-channel option is more advanced for the bender module as it takes cross-talk between channels into account. The guide module has the option of using a ballistic guide shape (see Section 2.4.1), while the bender module only models guides with cross-section that are either constant, or linearly decreasing or increasing.

Because the actual number of neutrons emitted from the source is very large ( $\sim 10^{15} \text{ s}^{-1}$ ), Vitess models the neutrons as a number of trajectories rather than individual neutrons. Each trajectory in Vitess is given a *weight*, normalized to represent neutrons per second. The user specifies the number of trajectories before the simulation. The larger the number of trajectories, the more realistic the output will be.

The weights will change when a trajectory undergoes reflection. Rather than the entire trajectory being reflected or transmitted at a boundary, it is assigned a new weight that represents the probability of reflection. The total weight of all trajectories at a point where they are detected corresponds to the neutron intensity at that point. This function was used to extract information about the lost neutrons in the Geant4 coupling, as described in Section 3.5.

### 3.3 Geant4 (GEometry ANd Transport)

Geant4 is an open-source simulation toolkit for particle transport that was developed at CERN. Geant4 was originally intended for high-energy physics but has found other applications, nuclear physics being one of them. Geant4 does not take into account diffraction effects of neutrons and therefore it cannot be used to simulate reflection of low-energy neutrons in guides. At ESS, it is used to investigate shielding of high-energy neutrons and the secondary particles that are created during scattering.

A simulation model in Geant4 is built as an application consisting of a number of classes, written in C++ code. The user builds the geometry of the problem and decides on which particles to use. Geant4 provides information about particles and how they are transported through materials. The information is stored in so-called physics lists, and the user chooses a physics list that contains information about processes that are relevant to the particles that are used in the simulations. The physics list used for this project is QGSP\_BERT, which contains information about the interactions of hadrons (e.g. neutrons). If simulation times are not an issue, a better physics list is QGSP\_BERT\_HP (HP stands for high precision), which provides detailed information about the cross-section for neutrons between thermal energies and 20 MeV.

The most common way to build a Geant4 application is by modifying one or several existing applications. Geant4 provides a large number of examples that can be used as a starting point.

The following classes are used to model the neutron guide in this project:

*PrimaryGeneratorAction.* Decides the energy, positions and direction of the primary particles that are sent in to the guide. Two different PrimaryGeneratorAction classes are used. The first models the signal from the ESS source. These neutrons are placed randomly at the start of the guide. The second source models the lost Vitess neutrons. A text file with the information of all particles is read at the start of each run. The class also sends some information about the primary particle (energy, momentum and position) to the class EventAction so that this information is saved if the particle is detected.

*DetectorConstruction.* Describes the geometry and material composition of the guide, shielding and detectors. The guide itself is made from copper, shielded by 1 meter of concrete. The neutron detector is rectangular and placed so that it covers the end of the guide. The gamma detector covers the entire outer surface of the shielding.

*RunAction.* Called at the beginning and end of each run. A run consists of a number of events. Creates the output file that is filled with information about detector hits at each event.

*EventAction.* One run consists a number of events. Each event starts with one primary particle. The function EndOfEventAction() fills the output file with particle information if a detector has a hit.

*NeutronSD.* Describes the functions of the neutron detector. The function ProcessHits() checks whether a particle that hits the detector is a neutron. If that is the case, it creates a NeutronHit object and inserts it into a hit collection.

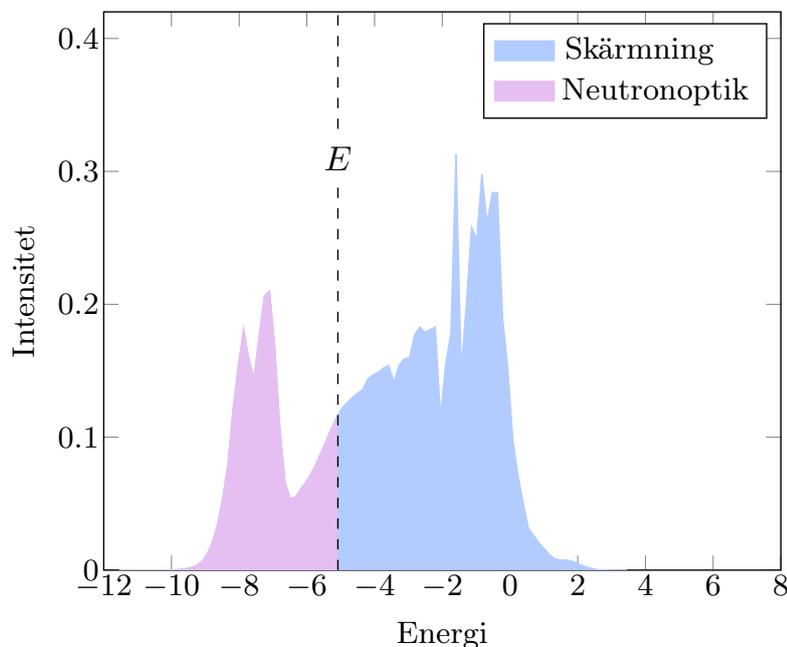
*NeutronHit.* Contains information about the neutron's kinetic energy.

*GammaSD.* Describes the functions of the gamma detector. Works in the same way as the neutron detector, but will only save gamma particles as hits. Both the particle's kinetic energy and its position are saved.

*GammaHit.* Contains information about the gamma particle's position and kinetic energy.

The output files created by Geant4 are ROOT files [23].

### 3.4 Simulation process



**Figure 3.2:** The energy spectrum of the neutrons coming from the ESS source. The spectrum was provided by the ESS neutronics group. From the ESS Technical Design Report [6].

The energy spectrum of the neutron produced at ESS covers a wide range of energies, as seen in Figure 3.2. The energy range that is most interesting for experiments is at the lower end of the spectrum, where the two high peaks correspond to neutrons from the cold and the thermal moderator. A typical simulation process using Geant4 and Vitess goes through the following steps:

1. Neutrons with  $E < E_1$  (see Figure 3.2) are modeled by Vitess. The *signal* consists of neutrons that are transmitted through the guide and are lower than some cut-off energy  $E_2$ . Transmitted neutrons that have higher energies are considered *noise*. In this project, the cut-off energy was 9 meV, or 3Å, meaning that the cold source was used.
2. Neutrons with  $E > E_1$  are modeled by Geant4. These neutrons will not be transmitted through reflection but might scatter and end up at the end of the guide. If detected, they contribute to the background noise.

After this process, there is one signal component and two noise components. The signal-to-noise ratio (SNR) is given by

$$\text{SNR} = \frac{(\text{signal})_V}{(\text{noise})_V + (\text{noise})_G}. \quad (3.1)$$

This project adds an extra step to the noise calculations by sending the non-transmitted neutrons from Vitess to Geant4. These neutrons will scatter inside the guide material or shielding. If the neutrons end up at the detector, they add to the noise according to

$$\text{SNR} = \frac{(\text{signal})_V}{(\text{noise})_V + (\text{noise})_G + (\text{noise})_{\text{coupling}}}. \quad (3.2)$$

### 3.5 Coupling Vitess and Geant4

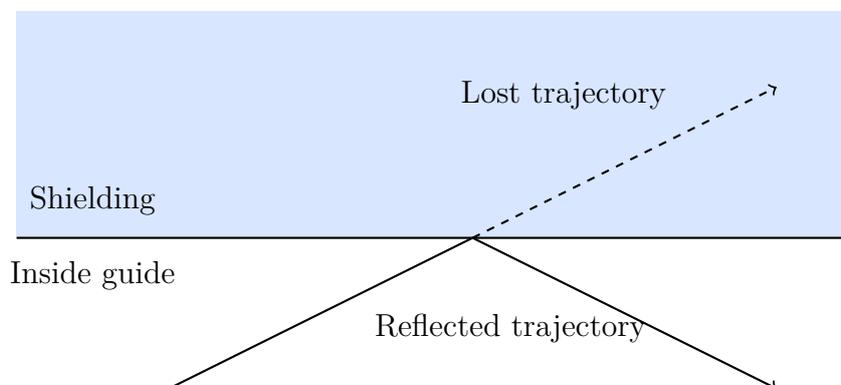
Vitess models a neutron beam as a collections of trajectories with different weights. At each boundary, the weight is changed due to the probability that neutrons of this particular angle and wavelength are reflected. The weight of the reflected trajectory is changed according to:

$$\text{weight}_{\text{new}}^{\text{refl}} = (\text{weight}_{\text{old}}) \cdot R, \quad (3.3)$$

$R$  being the reflectivity of the walls. This also means that a trajectory with weight

$$\text{weight}_{\text{new}}^{\text{trans}} = (\text{weight}_{\text{old}}) \cdot (1 - R), \quad (3.4)$$

is transmitted through the guide walls (Figure 3.3).



**Figure 3.3:** Reflection and transmission of a trajectory in Vitess.

The transmitted trajectories are considered lost by Vitess. However, there is still a chance that these neutrons will scatter in the shielding and reach the end of the guide, where they will contribute to the noise. They will also create gamma rays. To investigate this, a function was added to Vitess guide module code in order to save information about the lost trajectories - coordinates, energy, direction and weight. This information was then used to create a neutron source in Geant4.

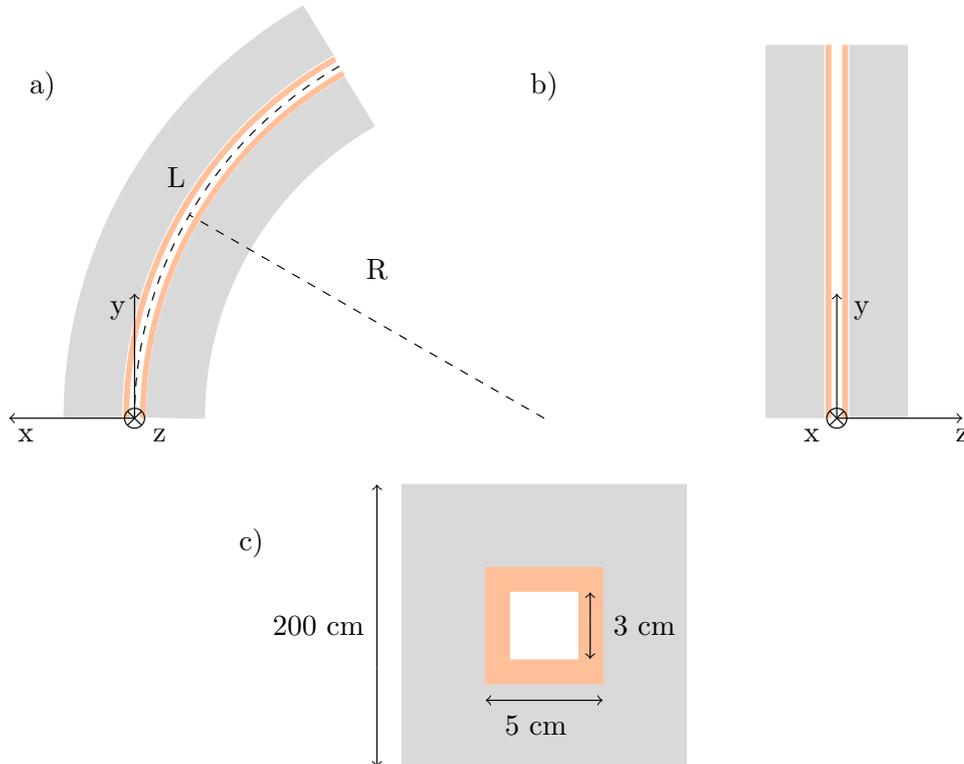
### 3.6 Geometry of the neutron guide for this project

This project uses a guide with a constant square cross-section of 3 cm x 3 cm, and length 4 m. It is curved along one direction. The tested curvatures were 1, 1.5, 2.0 and 2.5 times out of line-of-sight. The material for the guide is copper, which is a material with a large cross-section for high-energy neutrons. This is a simplified neutron guide - at ESS, copper will be used in combination with other materials to attenuate the high energy spectrum of neutrons (see Section 2.5). The guide is shielded by 1 m of concrete on all sides. Concrete is a standard material for neutron guide shielding.

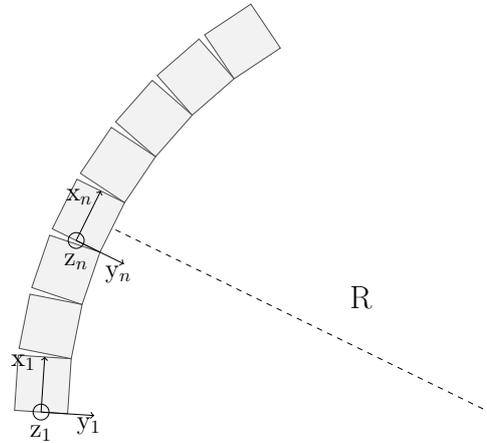
The Vitess guide and the Geant4 are not identical. Geant4 models the guide material and shielding, as seen in Figure 3.4. Vitess does not model the

shielding or guide material, only the thin supermirror coating inside the guide. The Vitess guide consists of straight segments, as seen in Figure 3.5. The coordinate systems are also different. The coordinate translation is described in Appendix A.

The radiuses of curvature were calculated using Equation 2.6. The  $m$ -values of the reflective coating were calculated using Equation 2.7, using a characteristic wavelength of  $3 \text{ \AA}$ . Because the guide used in this project was so short, the  $m$ -values calculated using Equation 2.7 would have to be impossibly high to transmit neutrons for 2.5 times out of line-of-sight. To combat this, the Vitess guide was split lengthwise into 6 channels, making the width of each channel  $a = 0.5 \text{ cm}$ . The radius and  $m$ -value for each curvature are shown in Table 3.1.



**Figure 3.4:** Neutron guide as modeled in Geant4. Not to scale. The outer shielding is concrete (gray), the guide itself is copper (orange) and inside the guide is vacuum (white). a) Top view; b) side view; c) cross-section.



**Figure 3.5:** Neutron guide as modeled in Vitess. The guide consists of straight segments. Each segment has a local coordinate system.

LOS	$R$ (m)	$m$
1.0	66.67	2.4
1.5	29.63	3.6
2.0	16.67	4.8
2.5	10.67	6.0

**Table 3.1:** Parameters for a 4 m neutron guide, with  $\lambda^* = 3 \text{ \AA}$ . First column: the curvature of the guide relative to a line-of-sight (LOS) guide.

A realistic neutron guide would not have such a large curvature in a short distance like 4 m. A guide that is 2 times out of line of sight would typically be 20 m or longer. The reason for choosing such a short guide is to cut down on simulation times and still get a reasonable amount of statistics in Geant4.

### 3.7 Normalization

The output from Geant4 needs to be translated to the unit neutrons/s in order to compare it to the output from Vitess.

### 3.7.1 Geant4 output

The output from Geant4 is a number of detector hits,  $N_{\text{hits}}$ . The outgoing neutron intensity  $n_{\text{out}}$  can be calculated according to

$$\frac{n_{\text{out}}}{n_{\text{in}}} = \frac{N_{\text{hits}}}{N_{\text{events}}} \longrightarrow n_{\text{out}} = n_{\text{in}} \cdot \frac{N_{\text{hits}}}{N_{\text{events}}}. \quad (3.5)$$

The intensity of neutrons entering the guide,  $n_{\text{in}}$ , depends on the size of the guide and its placement relative to the source. The neutron guide is placed at the distance  $d = 200$  cm from the source and the guide width is  $w_{\text{guide}} = 3$  cm (see Section 3.6). The horizontal angle  $\alpha$  between the source and the guide opening is

$$\alpha = 2 \arctan \frac{w_{\text{guide}}/2}{d} = 2 \arctan \frac{1.5 \text{ cm}}{200 \text{ cm}} = 0.859^\circ. \quad (3.6)$$

The following parameters are known:  $n_{\text{source}} \approx 3 \cdot 10^{15}$  neutrons/s is the neutron intensity from the source,  $\theta = 60^\circ$  is the angular opening for the neutron extraction area,  $h_{\text{guide}} = 3$  cm is the height of the guide opening and  $h_{\text{source}} = 12$  cm is the height of the neutron beam. Given these,  $n_{\text{in}}$  can be calculated according to

$$n_{\text{in}} = n_{\text{source}} \cdot \frac{h_{\text{guide}}}{h_{\text{source}}} \cdot \frac{\alpha}{\theta} = \frac{3 \text{ cm}}{12 \text{ cm}} \cdot 3 \cdot 10^{15} \cdot \frac{0.859^\circ}{60^\circ} = 1.07 \cdot 10^{13} \quad (3.7)$$

$$\longrightarrow n_{\text{out}} = 1.07 \cdot 10^{13} \cdot \frac{N_{\text{hits}}}{N_{\text{events}}}. \quad (3.8)$$

### 3.7.2 Geant4-Vitess coupling output

The original Vitess weight of each trajectory is one of the input parameters for the Geant4 coupling simulation. The weights of the detected particles

are saved in a vector (ntuple) in Geant4. Because the weights in Vitess are already normalized to represent neutrons per second, the weights of the detected particles are simply summed together to get the output in the correct unit. The weights are summed using a ROOT script.

# Chapter 4

## Results and discussion

### 4.1 Simulation process

A neutron guide was modeled in Geant4 and Vitess using the same parameters (see Section 3.6). Three different simulations were performed:

1. *Vitess*: Neutrons from the ESS source with lower energies than 8 eV / 0.1Å were simulated by Vitess. The moderator description file used was for the ESS cold source. The range of wavelengths was defined as 0.1 Å - 20 Å. The divergence of the source was set to be defined by a 3 cm x 3 cm window at a distance of 200 cm from the source (the guide opening). The number of trajectories were set to  $10^9$ .

The neutrons were either transmitted through the guide and detected at the end, or lost in the guide. Information about the lost neutron trajectories was saved in a data file. The detected neutrons were either counted as signal ( $\lambda > 3 \text{ \AA}$ ) or noise ( $\lambda < 3 \text{ \AA}$ ).

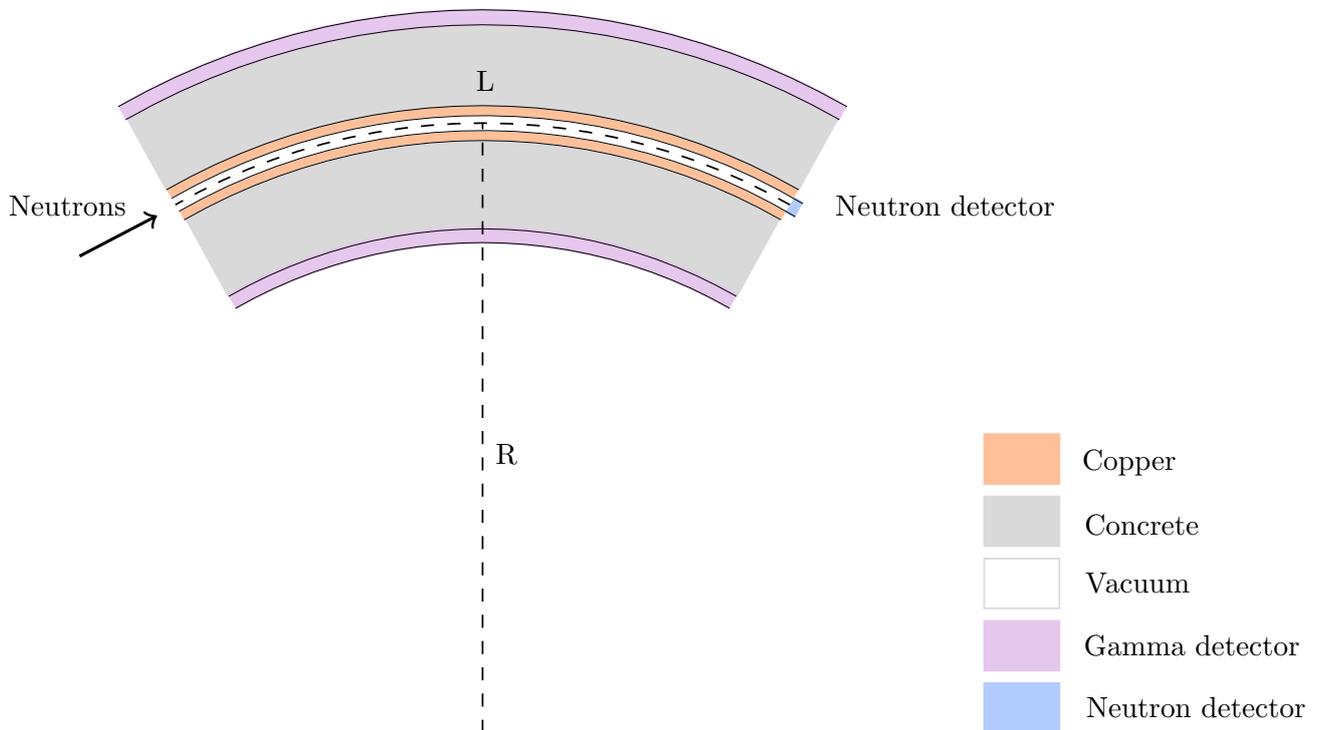
2. *Geant4*: Neutrons with energies above 8 eV were simulated by Geant4. The primary particles all started at the guide opening. The primary particles were all given the same momentum direction (in the y-direction, see figure 3.4). A Geant4 physics list for hadronic physics called QGSP\_BERT

was used. These simulations were run with  $2 \cdot 10^8$  primary particles on a multi-core computer using 20 threads. Typically, each simulation would run for a day.

All detected neutrons in these simulations contribute to the noise. Additionally, all gamma rays that escaped through the shielding were detected. The placement of the detectors are shown in Figure 4.1.

3. *Geant4*: Finally, simulations were run in *Geant4* using the data files from *Vitess* as a source. All of the neutrons that reached the detector were counted as noise. As in the previous step, gamma rays along the length of the guide were also detected. These simulations were faster than the first *Geant4* simulations and could be run without multi-threading.

Each simulation was performed for 4 curvatures, ranging from 1 to 2.5 times out of line-of-sight.



**Figure 4.1:** The neutron guide and detectors as modeled by *Geant4*.

## 4.2 Signal-to-noise ratio

The aim was to find the effect of the coupling term on the signal-to-noise ratio (SNR), which is a measure of signal quality.

LOS	Signal $S$ (neutrons/s)
1.0	$5.08\text{e}+11 \pm 7.12\text{e}+5$
1.5	$2.48\text{e}+11 \pm 4.98\text{e}+5$
2.0	$4.32\text{e}+10 \pm 2.08\text{e}+5$
2.5	$4.25\text{e}+9 \pm 5.85\text{e}+3$

**Table 4.1:** Signal levels at the end of the guide for different curvatures.

The signal  $S$  is defined as the neutrons with wavelength  $\lambda > 3 \text{ \AA}$ . The signal is shown in Table 4.1. The signal decreases for larger curvatures, which is expected as reflection becomes less likely when the incident angles of the neutrons increase (see Section 2.3). This signal decrease is what puts a limit on the curvature of the neutron guide - even if the signal-to-noise ratio will increase with larger curvatures, a small signal would be hard for the detector to pick up on which would result in long measurement times.

LOS	Noise $N_V$ , Vitess (neutrons/s)	Noise $N_G$ , Geant4 (neutrons/s)	Noise $N_C$ , coupling (neutrons/s)	Percentage of noise from coupling
1.0	$3.31\text{e}+10 \pm 1.82\text{e}5$	$(2.11 \pm 0.011)\text{e}+9$	$(3.0 \pm 0.13)\text{e}+6$	0.0085%
1.5	$1.43\text{e}+10 \pm 1.20\text{e}+5$	$(1.02 \pm 0.023)\text{e}+8$	$(1.22 \pm 0.014)\text{e}+8$	0.84%
2.0	$1.27\text{e}+9 \pm 3.56\text{e}+4$	$(5.1 \pm 0.53)\text{e}+6$	$(2.65 \pm 0.032)\text{e}+7$	2.04%
2.5	$(7.26 \pm 0.0085)\text{e}+5$	$(3.3 \pm 0.42)\text{e}+4$	$(1.62 \pm 0.013)\text{e}+6$	68%

**Table 4.2:** Noise levels at the end of the guide for different curvatures.

The three noise components are shown in Table 4.2.  $N_V$  is the noise from the Vitess simulation,  $N_G$  is the noise from the Geant4 simulation and  $N_C$  is the noise from the Vitess-Geant4 coupling. The Vitess noise component

$N_V$  dominates for all curvatures except the last one. The Geant4 noise component  $N_G$  gets smaller for increasing curvatures, as expected. The coupling noise component  $N_C$  is larger than  $N_G$  for all curvatures except the first. The coupling noise component stands out in the sense that there is no apparent trend. This component is largest for the 1.5 times out of line-of-sight guide. The reason for this could be that there are two competing effects. As the curvature increases, fewer of the simulated neutrons reach the end of the guide. On the other hand, a straighter guide has fewer reflections, which means there are fewer source particles in the coupling simulation.

In order to further investigate the importance of each noise component, three different signal-to-noise ratios were calculated:

$$\text{SNR}_1 = \frac{S}{N_V} \quad (4.1)$$

$$\text{SNR}_2 = \frac{S}{N_V + N_G} \quad (4.2)$$

$$\text{SNR}_3 = \frac{S}{N_V + N_G + N_C} \quad (4.3)$$

The results are shown in Table 4.3. Even though the signal decreases with larger curvatures (Table 4.1), the signal-to-noise ratio will increase. This is because more high-energy neutrons than low-energy neutrons will be stopped by the walls of the guide. The coupling effect gets more visible as the curvature of the guide increases, which is because the other two noise components are attenuated more when the curvature increases.

It would be interesting to use a larger detector that covers the end part of the shielding and not only the guide opening. Neutrons that are transmitted through the edge of the shielding may contribute to the background, depending on how the instrument or sample environment at the end of the guide is designed.

In the Geant4-only simulation, the source only illuminates the guide opening. A possible improvement would be to have the incident neutrons cover the side

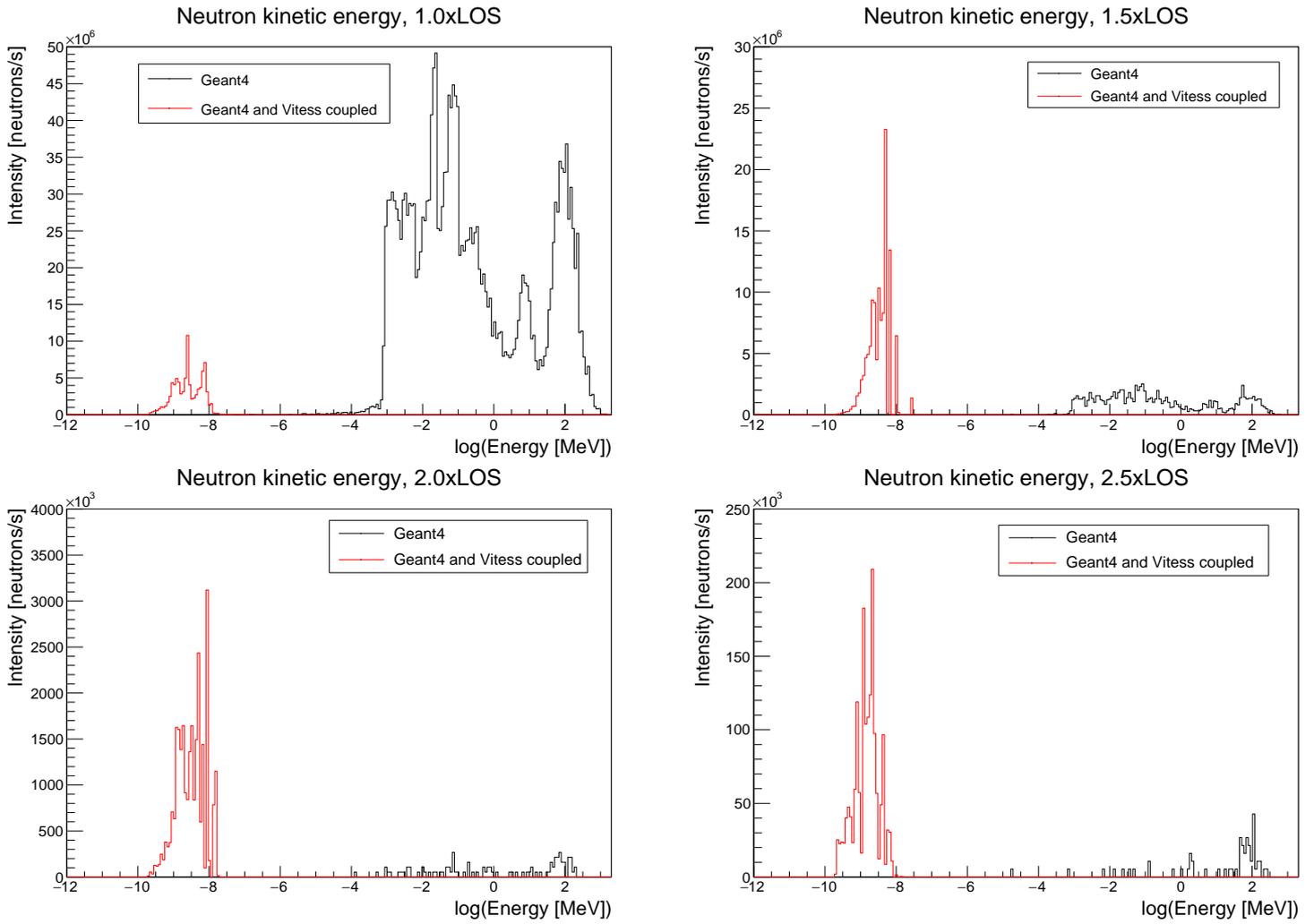
LOS	SNR, Vitess only	SNR, Vitess and G4 separately	SNR, with coupling term
1.0	$15.33 \pm 8.70\text{e-}5$	$14.43 \pm 0.0043$	$14.43 \pm 0.0043$
1.5	$17.34 \pm 1.50\text{e-}4$	$17.22 \pm 0.0028$	$17.08 \pm 0.0032$
2.0	$34.02 \pm 9.68\text{e-}4$	$33.88 \pm 0.014$	$33.19 \pm 0.016$
2.5	$5854 \pm 6.87$	$4040 \pm 1.39$	$1591 \pm 26$

**Table 4.3:** Signal-to-noise ratios for different curvatures.

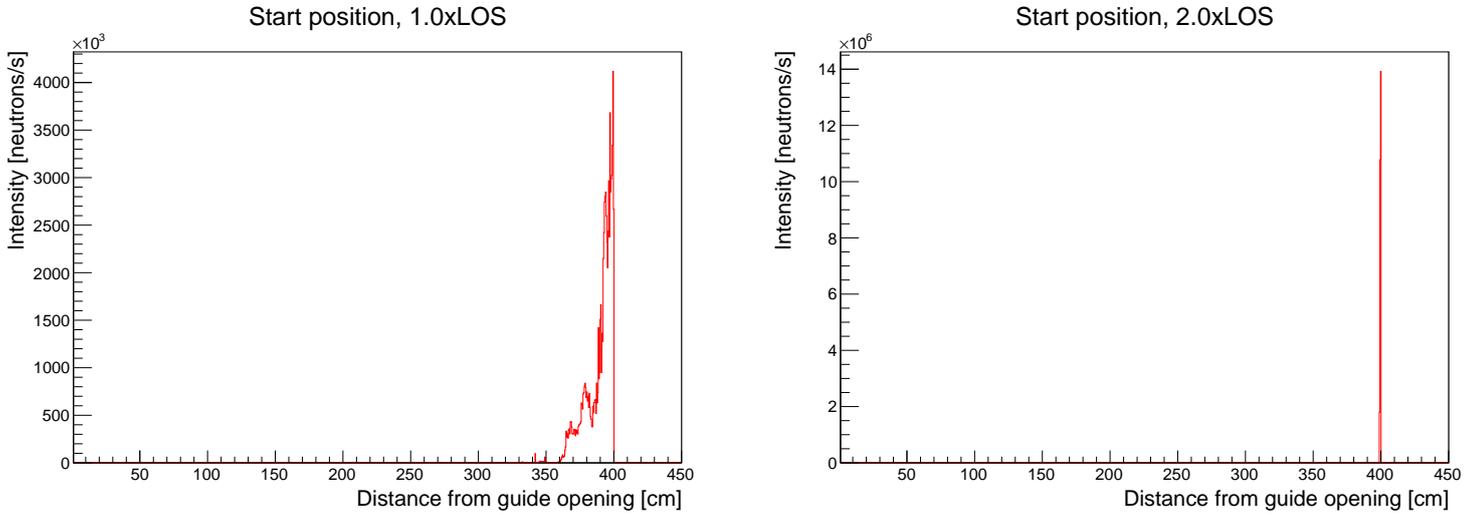
of the shielding as well. In that case the second noise component ( $N_G$ ) might have been larger.

Figure 4.2 shows how the energy of the neutrons from the Geant4-Vitess coupling compares to the neutrons from the Geant4-only simulation. It is shown that the intensity of the noise from the coupling is comparable to the noise at large curvatures. However, the energies of the coupled neutrons are significantly smaller, ranging from about 0.1 meV to 0.1 eV.

The coupled neutrons have starting positions all throughout the guide. The likelihood of them being detected increases as they get close to the detector, which is placed at the end of the guide (see Figure 4.1). The starting positions of the detected neutrons for two different curvatures (1 and 2 times line-of-sight, respectively) are shown in Figure 4.3. Both plots show that a majority of the starting points are in the last part of the guide, especially for the 2 times out of line-of-sight guide where the neutron trajectories all start at the very edge of the guide. This suggests that only the very last part of the guide needs to be simulated for the coupled noise component, which would reduce simulation times. Furthermore, in order to reduce this noise, the modifications to the neutron instrument would be focused to the end of the guide.



**Figure 4.2:** Energy distribution of detected neutrons at the end of the guide.



**Figure 4.3:** Start position of the trajectories that are detected at the end of the guide. The guide length is 400 cm. Left: Line-of-sight guide. Right: 2 times line-of-sight guide.

### 4.3 Gamma rays

Gamma rays are high-energy photons that are emitted when neutrons are captured or scattered by atoms. Gamma rays are ionizing radiation that are biologically hazardous in high doses. The gamma detector in this example covers the full length of the shielding surrounding the guide, in order to investigate the gamma rays that escape through the shielding (see Figure 4.1).

The number of detected gamma particles for the Geant4 simulation and the coupled simulation are shown in Table 4.4. The gamma particles from the coupled simulation constitute about 20% of the total count, with the exception of 1 times line-of-sight guide.

The energy distributions of the gamma rays are shown in Figure 4.4. The coupled spectrum has a maximum energy of 7-8 MeV. This energy marks a typical neutron binding energy, which suggests that the gamma rays in the coupled simulation are created mainly by neutron capture.

LOS	Gamma particles, only Geant4 (particles/s)	Gamma particles, Vtess and Geant4 coupled (particles/s)	Percentage of gamma particles from coupling
1.0	$1.92\text{e}+10 \pm 3.31\text{e}+7$	$(2.31\text{e}+7 \pm 7.32\text{e}+5)\text{e}+7$	0.12%
1.5	$(2.04 \pm 0.010)\text{e}+9$	$(5.41 \pm 0.048)\text{e}+8$	20.96%
2.0	$(2.07 \pm 0.011)\text{e}+9$	$(5.72 \pm 0.050)\text{e}+8$	21.65%
2.5	$(2.07 \pm 0.0033)\text{e}+9$	$(5.17 \pm 0.032)\text{e}+8$	19.98%

**Table 4.4:** Detected gamma particles for different curvatures.

The spatial distribution of gamma rays along the guide is shown in Figure 4.5. There is a downward slope towards the end, most likely because the numbers of neutrons decrease along the guide.

The guide material used in these simulations was copper. It would be interesting to investigate the gamma ray levels for a boron-containing material, which is commonly used in neutron guides to absorb unreflected thermal neutrons. Boron's high neutron capture cross-section at thermal energies would lead to higher levels of gamma particles compared to these simulations.

These simulations were run using the Geant4 physics list QGSP\_BERT. Figure 4.6 shows the plot for a test run with the coupled neutrons using the more precise physics list QGSP\_BERT\_HP. Compared to the QGSP\_BERT run, there were actually fewer gamma particles created although the gamma particles had slightly higher energies.

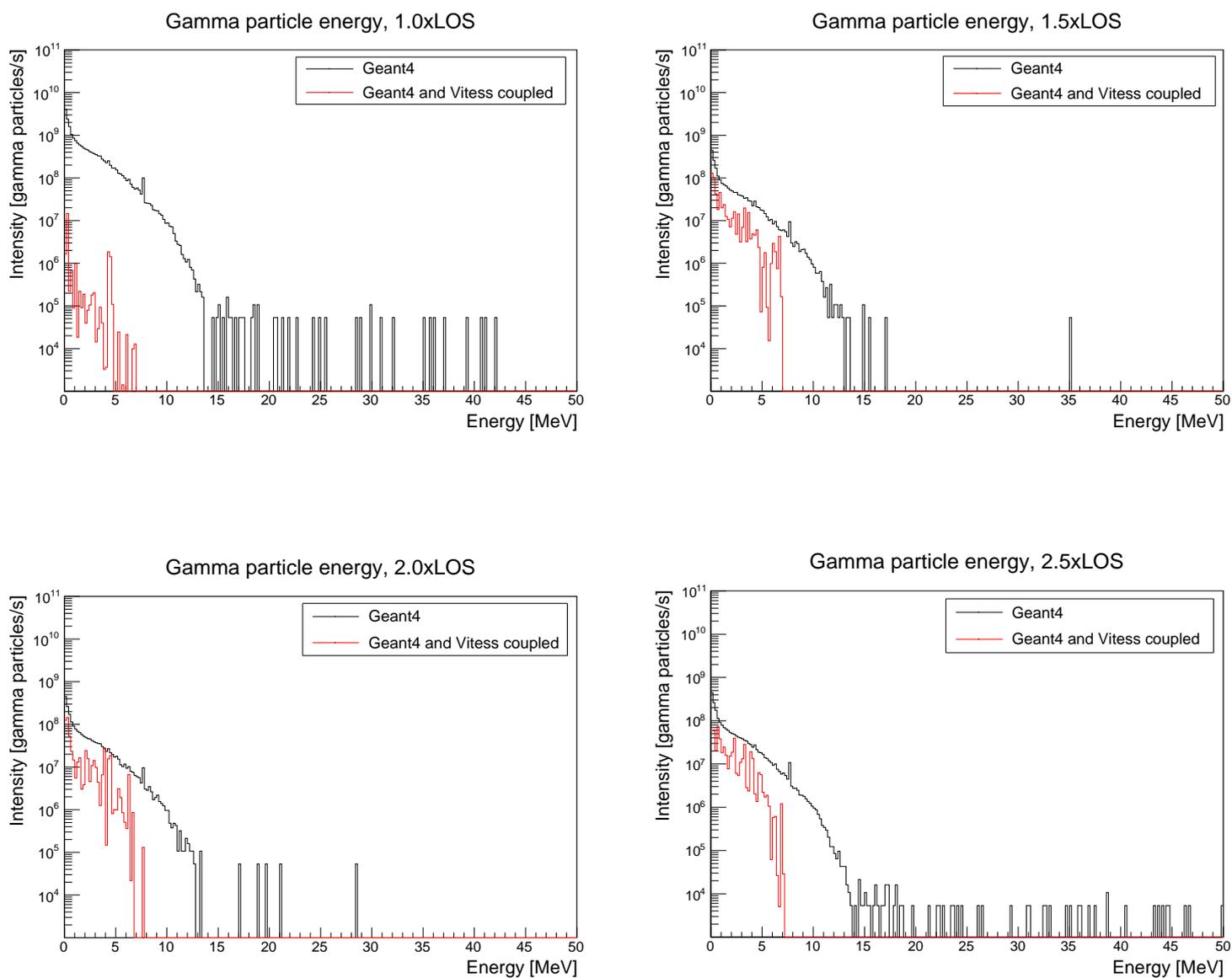
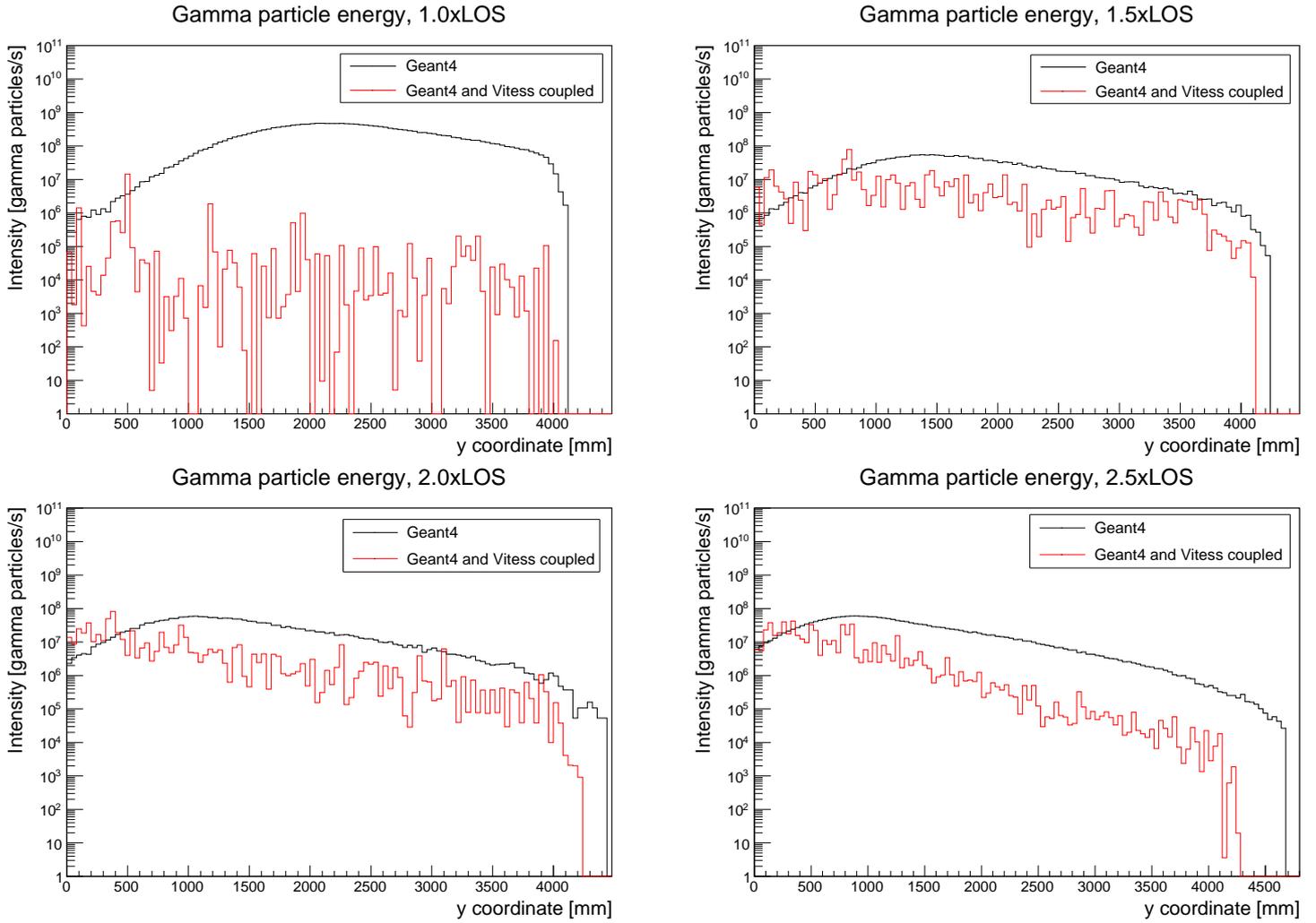
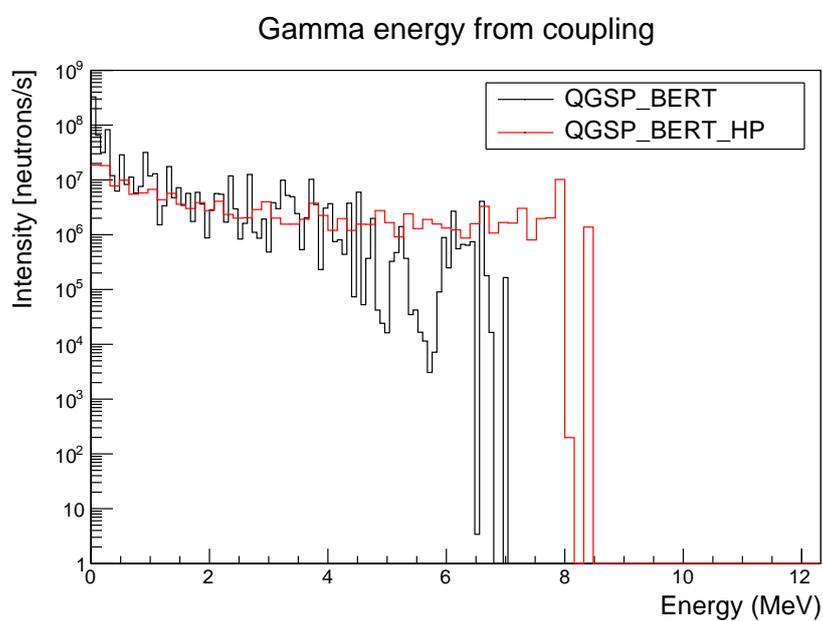


Figure 4.4: Energy distribution of the detected gamma rays.



**Figure 4.5:** Position along y-direction of the detected gamma rays.



**Figure 4.6:** Comparison between 2 different physics lists in Geant4 (1.5 times line-of-sight).

# Chapter 5

## Conclusion

The method proposed in this thesis shows a simple way couple Vitess to Geant4 by extracting information from Vitess and using it to create a source in Geant4.

The method was tested for a neutron guide model. The neutrons from the coupling that hit the detector were added to the background noise, which affected the signal-to-noise ratio. The results from the example suggest that the coupling does have an impact on the signal-to-noise ratio, especially as the guide curvature increases. The neutrons from the coupling have kinetic energies between 0.1 meV and 0.1 eV. The coupled neutrons will also produce gamma particles with energies up to 8 MeV.

### 5.1 Outlook

The neutron guide used to test the coupling in this project was simplified in order to make the simulation times shorter. To further test the coupling effect, a more realistic guide could be designed:

- The guide could be longer, 20 meters or more. A real guide that was 2 times out of line-of-sight would not be as short as 4 meters.

- The HP physics list in Geant4 should be used. This makes simulation times longer, but gives more accurate predictions as it takes the varying neutron cross-section into account.
- For the Geant4-only simulation, the primary particles were concentrated to the guide opening, but could perhaps have been distributed over the side of the guide walls and the shielding as well. Also, the simulated neutrons all had the same momentum direction. It is possible to give the primary neutrons slightly different directions in order match the beam divergence of the ESS source.
- The supermirror coating could be included in Geant4. The thin layers with many reflections are a significant source of gamma rays.
- Using a boron-containing material in the guide would probably also increase the amount of gamma rays.

The Vitess guide could also match the Geant4 guide more closely. Either by using a different geometric shape in Geant4 or by using the bender module instead of the guide module in Vitess. Before using the bender module the code for it would have to be modified to export lost neutrons, like the guide module was modified in this project. Only the Vitess guide used channels in this project but these could be added to the Geant4 guide as well, especially used in combination with supermirror coating.

The neutron detector was placed so that it covered the end opening of the guide, but it could also had been placed to cover the end part of the shielding.

In this project, the gamma rays were investigated in relation to radiation safety, which is why the detected gamma rays were the ones that escaped along the guide. A gamma detector could also be placed at the end of the guide, which would be more relevant for investigating gamma background in instruments.

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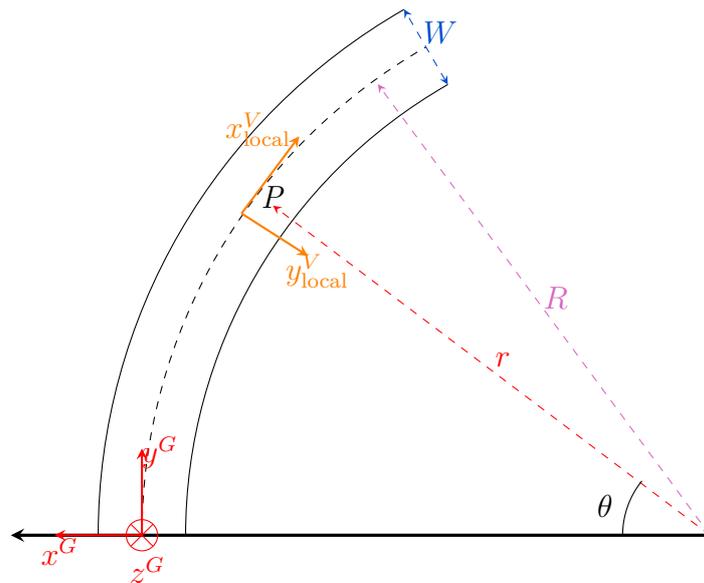
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# Appendix A

## Translating coordinates



**Figure A.1:** The curved guide as it looks in Geant4. The Vitess coordinate system (orange) is aligned with the guide segment in Vitess.

The Vitess guide is made up of straight segments, each with a local coordinate system. The Geant4 guide is curved.

First, the local coordinates for a guide segment in Vitess  $\{x^V_{\text{local}}, y^V_{\text{local}}, z^V_{\text{local}}\}$

are translated to  $\{x^V, y^V, z^V\}$ :

$$x^V = x_{\text{local}}^V + ((\text{segment number}) - 1) \cdot (\text{segment length})$$

$$y^V = y_{\text{local}}^V$$

$$z^V = z_{\text{local}}^V$$

Translating  $\{x^V, y^V, z^V\}$  to  $\{x^G, y^G, z^G\}$  is like mapping a straight guide to a guide of the same length that is curved with the radius of curvature  $R$ . The angle  $\theta$  in the figure is

$$\theta = \frac{x^V}{R}.$$

The radius of a point  $r$  is

$$r = R - y^V.$$

Given  $r$  and  $\theta$  for a point, the coordinates  $\{x^G, y^G, z^G\}$  can be calculated:

$$x^G = -1 \cdot (R - r \cos \theta)$$

$$y^G = r \sin \theta$$

$$z^G = -z^V$$

# Appendix B

## Summary in Swedish

### Kopplad datorsimulering av neutronoptik och skärmning för neutroninstrument på ESS

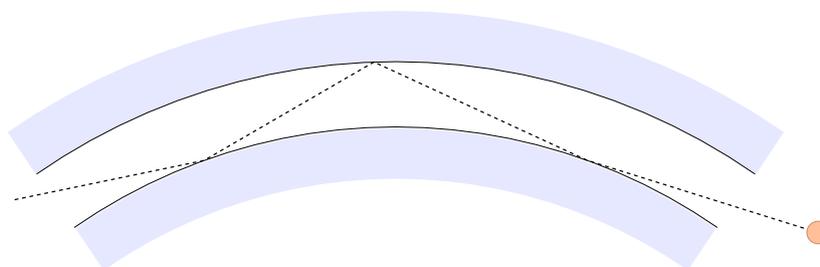
*När den här rapporten skrivs har forskningsanläggningen European Spallation Source (ESS) börjat byggas i Lund. ESS förväntas bidra till nya upptäckter inom många olika ämnen, till exempel materialforskning, medicin, partikelfysik och arkeologi. I det här projektet har jag undersökt hur datorsimuleringar av neutronflödet på ESS skulle kunna förbättras genom att koppla ihop två simuleringsprogram som är specialiserade på neutronoptik respektive skärmning av neutroner.*

ESS kan liknas vid ett avancerat mikroskop som kan användas för att undersöka mycket små strukturer. Metoden kallas neutronspridning (*neutron scattering* på engelska). Genom att låta neutroner studsas mot atomkärnorna i ett material går det att bygga upp en bild av hur materialet ser ut på atomnivå.

För att göra exakta mätningar är det viktigt att neutroner med rätt energi används. Utformningen av instrumenten som väljer ut och styr neutronerna utgår från två viktiga koncept - neutronoptik och skärmning. Neutronoptik består av optiska komponenter som väljer ut neutroner med rätt energi och styr dem till platsen för mätningen. Skärmning (eng. *shielding*) består av

material som stoppar neutroner med hög energi som annars riskerar att störa mätningarna. Skärmning är också viktigt för att stoppa den gammastrålning som bildas när neutronerna kolliderar med atomkärnor.

Neutronoptik utgår från att neutroner beter sig som vågor. Precis som ljusvågor kan neutroner manipuleras med optiska komponenter, till exempel linser och speglar. Figur B.1 visar en optisk komponent som kallas för neutronguide. Den består av ett rör med innerväggar som behandlats för att reflektera neutroner. Neutronerna transporteras framåt i neutronguiden genom att studsas mellan väggarna. Detta liknar hur ljus transporteras genom optiska fibrer.



**Figure B.1:** Neutron som transporteras genom en neutronguide.

Neutroner med låg energi har större sannolikhet att reflekteras än neutroner med hög energi. Neutronguiden har därför två funktioner - att styra neutronerna till rätt plats, och att sortera bort bakgrundbrus i form av neutroner med hög energi. Neutroner som inte reflekteras kommer att försvinna ur guiden genom väggarna och måste stoppas med skärmning för att förhindra att de tar sig till mätningarna på annan väg.

För att designa instrument som ger så lite bakgrundbrus som möjligt behövs datorsimulering. I regel utförs simuleringen i två omgångar. Först använder man ett program som simulerar hur neutronoptiken påverkar neutroner med låg energi. Sedan används ett annat program som simulerar hur skärmningen stoppar neutroner med hög energi. För att kunna dela upp simuleringen såhär måste man anta två saker: att neutroner med hög energi inte kommer reflekteras i neutronguiderna, och att neutroner med låg energi inte behöver skärmas. Risken är att denna metod är alltför förenklad, och att vissa neutroner kan behövas undersökas med båda programmen.

I mitt projekt tittade jag på om skärmningen behöver modifieras för att

inkludera neutroner med låg energi. Detta undersöktes genom att göra en koppling mellan två program. Det visade sig att skärmningen inte stoppade allt bakgrundsbrus som bestod av neutroner med låg energi. Andelen av det totala bakgrundsbruset som utgjordes av dessa neutroner var oftast liten, men kunde bli större beroende på neutronguidens utformning. Dessutom ökade den uppmätta mängden gammastrålning med ungefär 25% när man använde sig av kopplingsmetoden. Min slutsats är att det är nödvändigt att inkludera en koppling mellan simuleringarna för att få en komplett bild av bakgrundbruset och gammastrålningen.