

**COURSE: INTRODUCTION TO NEUTRON SCATTERING EXPERIMENTS AT  
LARGE SCALE FACILITIES.**

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This work entails a report of activities undertaken during the courses and seminars of the Introduction to neutron scattering experiments at large scale facilities. It covers a brief introduction on neutrons, X-rays and neutron scattering. Then a description of the VITESS software package summarized, including an example chosen for demonstration purposes – which is based on some aspects of Neutron spectrometer development.

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## Chapter 1

### Introduction

Even though he is not the first to have observed their effects; German physicist Wilhelm Röntgen is typically credited for the discovery of X-Rays in 1895 because he was the first to comprehensively study them. He was experimenting with vacuum tubes when he noticed the invisible light, which was covered with a black cardboard capable of stopping all visible light [1].

Having reasoned that the vacuum tube was giving off invisible rays Röntgen conducted a series of well-thought experiments in which he found that these rays could penetrate through certain objects but not others. Such as being able to pass through soft human tissue but unable to penetrate solid bone tissue.

On the other hand, a few decades later, in 1930, Walther Bothe and Herbert Becker performed an experiment, which was further improved by Irène and Frédéric Joliot-Curie. They, however, misinterpreted their results and believed to have observed  $\gamma$ -rays while they had seen neutrons.

After additional experimental verifications, James Chadwick gave the correct interpretation of these experiments in 1932. James Chadwick demonstrated that the interpretation of the experimental results was incompatible with energy and momentum conservation, if one accepted the  $\gamma$ -quanta hypothesis. One of his arguments was the following: if Be emits  $\gamma$ -rays, then the observed reaction would be:



He observed that the mass defect of  ${}^{13}\text{C}$  is known with sufficient accuracy to show that the energy of the [photon] emitted in this process cannot be greater than about 14·106 volts. It is difficult to connect such a quantum to the effects observed. Chadwick demonstrated that it may be assumed that the radiation consists of particles of mass 1 and charge 0, or 'neutrons'. Indeed, if the reaction is



there is plenty of energy left for the neutron [2].

Immediately, the new particle, the neutron, became essential for nuclear and elementary particle physics. It entirely changed the whole research landscape. Enrico Fermi and his group applied it to artificial radioactivity, substituting neutrons to  $\alpha$ -rays initially used by Joliot-Curies. They also discovered that slow neutrons were more efficient than fast ones in certain nuclear reactions. A decade later strong Neutron Sources in the form of Fission Reactors became available [3].

### Neutron Scattering

This is a powerful tool to probe dynamic and static properties of condensed matter at microscopic levels – in which the events are described by means of energy and momentum transfer. There are two types of neutron scattering namely, elastic and inelastic scattering.

Elastic scattering is involved in the investigation of a static structure whereby the energy of the neutron does not change. In contrast, in inelastic scattering the energy of the neutron changes and is involved in the investigation of the dynamic structure excitation in condensed matter [4].

That means there is an energy exchange between the neutron and the sample. These interactions are measured with cross section. We describe the interaction of a neutron beam with materials by introducing the central concept of cross sections. Thus, we define the flux of a neutron beam as the neutron rate per area:

$$\Psi = \frac{\text{Number of neutrons impinging on a surface per second}}{\text{Surface area perpendicular to the neutron beam direction}} \quad (3)$$

usually given in the unit  $n/(cm^2s)$

The *neutron scattering cross section*,  $\sigma$ , of a system is defined by the system's ability to scatter neutrons:

$$\sigma = \frac{1}{\Psi} \text{Number of neutrons scattered per second} \quad (4)$$

For a single nucleus,  $\sigma$  can now be seen as the effective area of the nucleus perpendicular to the neutron beam. The scattering cross section used here is the total cross section, which depends on the system (sample) volume,  $V$ . For thin samples,  $\sigma$  can be described by the volume specific cross section,  $\Sigma$ , through

$$\sigma = V\Sigma \quad (5)$$

The angular dependence of the scattered neutrons is the most important aspect of all neutron scattering [5]. To describe this dependence, we define the *differential scattering cross section* as the intensity of neutrons scattered into a particular solid angle,  $d\Omega$ . We denote the wave vector of the incoming neutron by  $k_i$  and that of the outgoing neutron by  $k_f$ , where the indices "i" and "f" denote *initial* and *final*, respectively. This is illustrated in Figure 1 and is quantified as:

$$\frac{d\sigma}{d\Omega} = \frac{1}{\Psi} \frac{\text{number of neutrons scattered into a solid angle } d\Omega \text{ per second}}{d\Omega} \quad (6)$$

The total number of scattered neutrons is the integral of neutrons per solid angle over all of the  $4\pi$  solid angle, hence

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega \quad (7)$$

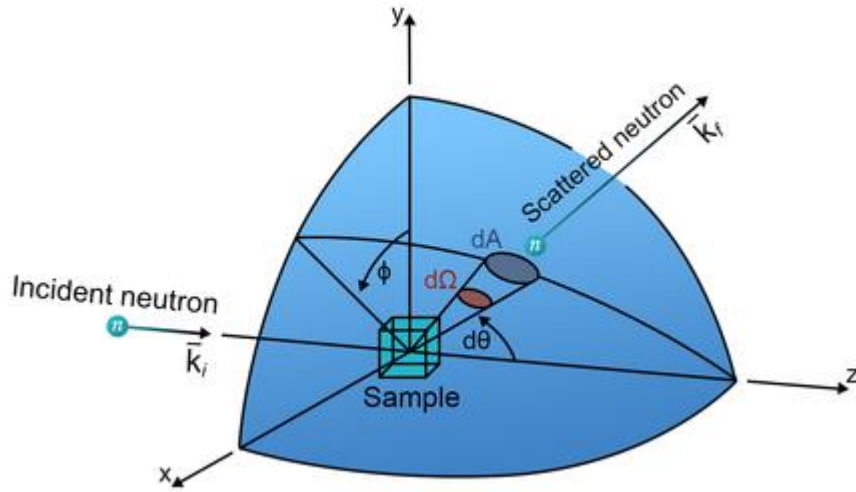


Figure 1: An illustration of the scattering geometry. The incoming neutrons, labelled  $k_i$ , scatter at the center of the sphere with the scattering angle  $2\theta$  and azimuthal angle  $\phi$ . The neutrons scattered into the solid angle element  $d\Omega$  (or detector area  $dA$  or labeled with  $k_f$ ).

Neutrons are scattered by the nuclei, meaning the strong nuclear forces. The range of these forces are femtometers (fm), much smaller than the neutron wavelength (measured in  $\text{\AA}$ ). Thus, the neutron cannot probe the internal structure of the nucleus, and the scattering from a single nucleus is isotropic [6].

## VITESS Software package

Analytical approaches have a limited role to play in complex experimental situations, such as neutron scattering. Even if most individual instrument components can be precisely described by analytical models, the integration of many such components in an instrument makes analytical processes highly inefficient and time consuming. Monte Carlo (MC) simulation offers an efficient solution for achieving this goal, both in terms of computational time and the time invested by researchers, given that powerful program packages, such as VITESS, are available [7].

Initially, VITESS was developed for the European Spallation Sources (ESS) Project [8]. It was used to simulate large parts of the "instrument suite" for the evaluation of these instruments of the long pulse spallation source (LPSS) partly in comparison to instrument at other sources. This aims at the optimisation of moderator-instrument performances.

Simulation of neutron scattering instruments is important for the development of new beamlines or update of existing instruments by enabling tests of new ideas and optimization of instrument components prior to construction. It can further be useful to conduct a virtual experiment to prepare a planned measurement, analysing data obtained by a simulation of the instrument in the foreseen configuration including an adequate description of the sample and detector output [9].

VITESS is an open-source software available on the VITESS website for Windows, Linux und Macintosh. It is mainly developed at the Helmholtz-Zentrum Berlin (formerly Hahn Meitner-Institut) in Germany but also includes contributions made by advanced users from other facilities.

## Software Concept and Layout

Monte Carlo ray-tracing technique [10] is used by VITESS, whereby neutrons are modelled as trajectories travelling from a source through an instrument onto a sample in which they are scattered and thereafter measured in a detector. They are assigned with a weight which corresponds to the intensity of the particular phase space element and ensures that the flux normalisation throughout the instrument is always correct independent of the number of generated trajectories. This weight is modified at each interaction with various instrument components.

Each component is represented by a module coming as a stand-alone executable in the software package [11]. These modules run independently of each other, with each single module reading in neutrons from the previous one and passing them on to the next one. A whole instrument is simulated by running several modules sequentially in a pipe. This is done in packages of 10000 neutrons such that in a simulation with larger statistics as usual, all modules can run simultaneously. The properties of generated neutron trajectories can be examined by monitors at any point in the instrument or written to a file to be read in again later by a new simulation continuing the instrument.

In addition, a Graphical User Interface (GUI) is utilized by VITESS from which an instrument can easily be built by assembling the needed modules and which allows to perform complex simulations without knowledge of any scripting language. A VITESS simulation can however also be run either directly from the command line or via a shell, python, perl or tcl script to which an instrument description can be exported from the GUI. This can also be used to run VITESS on a computer cluster, and since release 3.1, a framework is provided to split the simulation on a cluster into several instances to save simulation time.

## Chapter 2

The fundamental purpose of Neutron guides is to increase the neutron flux at the sample position. They were introduced in 1963 and evacuated to prevent neutrons scattering with air molecules, and the low divergent neutrons hitting the neutron guide walls at low grazing angles were reflected and transported more efficiently.

Most materials have a refractive index that is slightly below 1 for cold and thermal neutrons, hence there is a critical angle,  $\theta_c$ , below which there will be total external reflection of the neutrons, as demonstrated by Fermi and co-workers [12].

The critical angle is given by:

$$\sin \theta_c = \lambda \sqrt{\frac{Nb}{\pi}} \quad (8)$$

where  $N$  is the atomic number density of the material and  $b$  is the average coherent neutron scattering length.  $Nb$  is referred to as the neutron scattering length density.

Natural nickel (Ni) has one of the highest neutron scattering length densities of the elements in the periodic table which has a critical angle defined as  $m=1$ . To reflect neutrons at still higher angles than that corresponding to  $m=1$ , one could use the  $^{58}\text{Ni}$  isotope. This has a higher neutron scattering length density compared to Ni, equivalent to  $m=1.18$ .

Another option is to use supermirrors, proposed by Mezei [13] in 1970s, and which today can be made with  $m$ -values above  $m=7$ . Neutrons that are not reflected by the coating will be transmitted, and will be absorbed in the coating or in the substrate. Most neutron absorption processes cause the emission of gamma radiation, and the quantity and energy of the photons depend on the absorbing atom. The substrates for most neutron guides are made of glass that contains boron, and the products "borofloat" and "borkron" are common. Natural B contains 20% of the isotope  $^{10}\text{B}$ , which has a very high absorption cross section for cold and thermal neutrons. When a neutron is absorbed in  $^{10}\text{B}$ , the majority of the emitted gamma radiation is at a relatively low in energy (0.477 MeV).

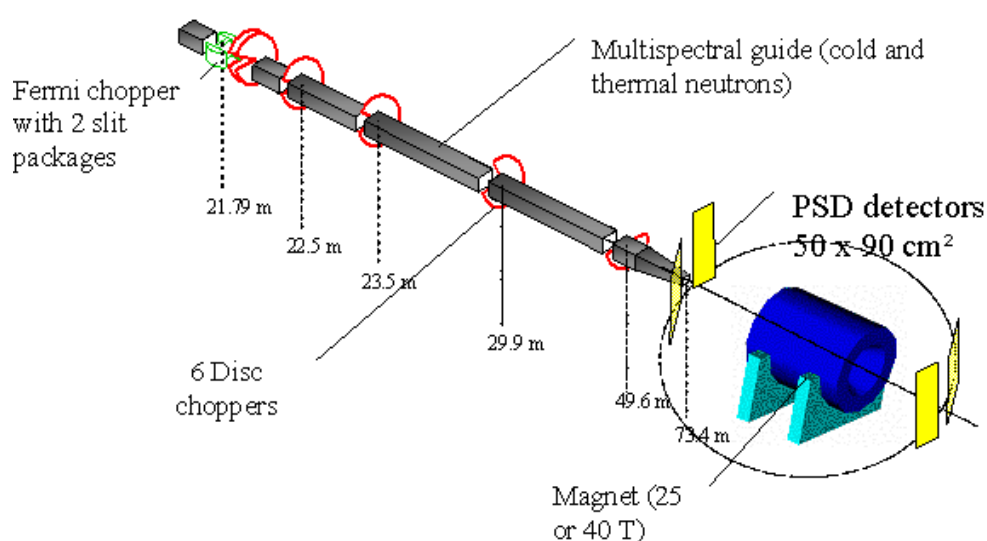


Figure 2: Schematic view of the EXED instrument. The grey tubes correspond to a ballistic neutron guide. The neutron pulses are produced alternatively by a Fermi chopper (in green) or by a counter rotating double disk chopper (in red), which are exchangeable. The other disk choppers (in red) are frame overlap choppers and a wavelength band chopper. The position sensitive gas detectors are presented in yellow and can be moved around the sample and the magnet.

## Example of VITESS application

The chosen example to demonstrate application of VITESS involved the running of the software to compare of the ballistic guide outputs under different parameters such as changing the source moderator. Also, software was run executed whereby the bottom plane of the guide was not coated and compared to when all planes of the guide were coated.

The Ballistic Guide example on VITESS:

Details: Source: A disc with 12 cm diameter emitting a constant (with wavelength) spectrum, 150 cm distance to guide. Guide dimensions: 6x6 cm<sup>2</sup> cross section at start, 12x12 cm<sup>2</sup> cross section after 5 m until 15 m, 6x6 cm<sup>2</sup> cross section at 20 m. Monitors: 2D Position, two 1D (y & z) position monitors, 2D divergence, wavelength monitor at 150cm after guide exit.

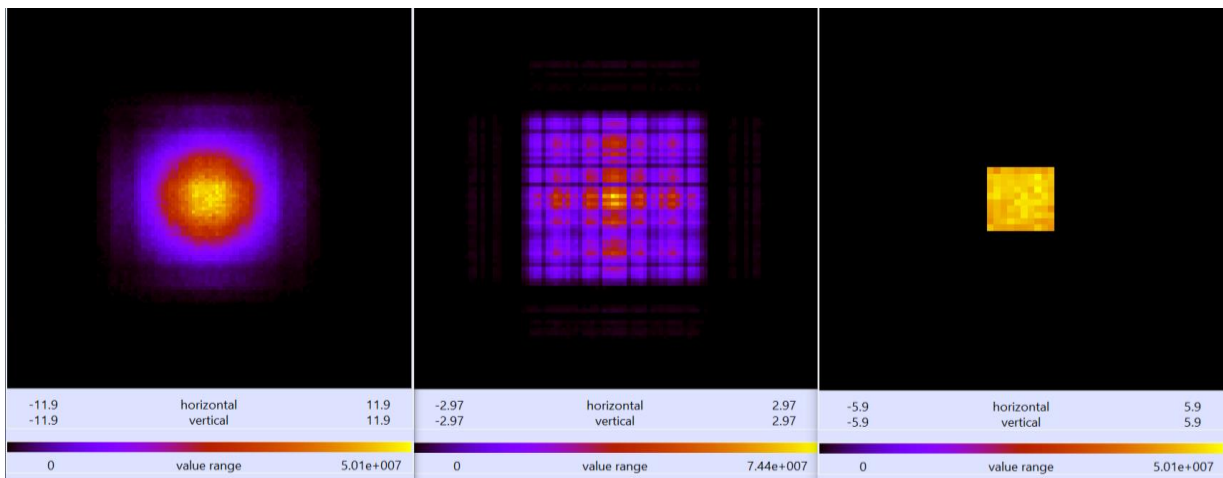


Figure 3: Visualizations of the neutron beam intensity at the position monitor 2D, divergence monitor 2D and monitor after the slit – with a constant source and bottom plane of the guide not coated.

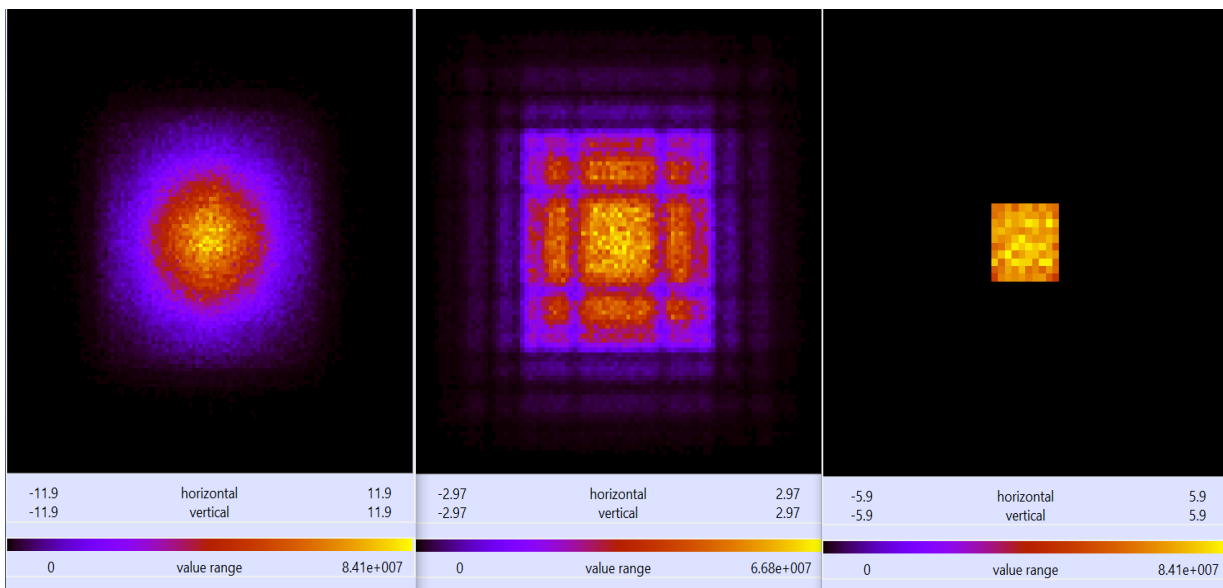


Figure 4: Visualizations of the neutron beam intensity at the position monitor 2D, divergence monitor 2D and monitor after the slit - with a Reactor cold source and all planes of guide coated.



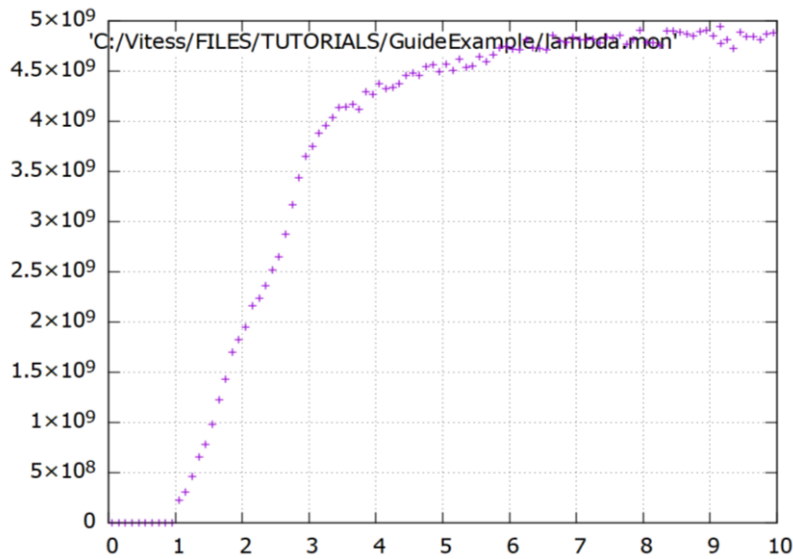


Figure 5: Lambda monitor plot of the beam profile as a function of wavelength, with the wavelength range from 0 – 10 (Å) with a constant neutron source.

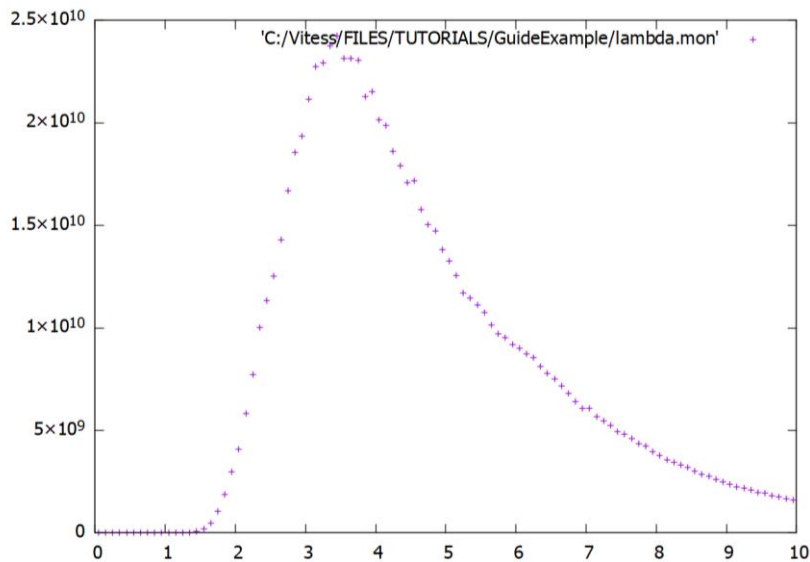


Figure 6: Lambda monitor plot of the beam profile as a function of wavelength, with the wavelength range from 0 – 10 (Å) with a ReactorCold.mod neutron source.

## Conclusions

The use of neutron guides is fundamental in increasing neutron flux, and it was demonstrated through the VITESS simulations. Comparing the visualizations (Figure 3 & 4) of the beam intensities, when the source and coating parameters are varied clearly shows that the beam intensifies with more coating of all planes of the ballistic guide. Both the 2D monitors and 2D divergence visually proves this point, including monitor after the slit. Definitely with many trajectories, better results can be achieved.

Another testimony that VITESS is a powerful tool, is the difference in figure 5 & 6 whereby the beam profiles are compared at the lambda monitor just before the slit. With the neutron yield peaking at lower wavelengths  $\sim 3.5$  Å on the latter, indicated by the classic gaussian curve. The former, indicates a peak of neutrons at larger wavelengths and a lower yield.

Neutron spectrometer development it is strongly linked to the Monte Carlo simulation software packages (VITESS, McStas etc.) for a better performance and evaluation of the parameters.

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