JOINT INSTITUTE FOR NUCLEAR RESEARCH
Frank Laboratory of Neutron Physics

FINAL REPORT ON THE INTEREST PROGRAMME

Monte-Carlo simulation of neutron scattering experiment

Supervisor:
MSc. Marta Klepacka

Student:
Mostafa Elnaggar, Italy,
University of Pisa

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Abstract

Mcstats is a Neutron scattering ray-tracing simulation tool which uses the Monte-Carlo method. It will be used to simulate NERA which is an indirect geometry spectrometer designated predominantly for the study of molecular dynamics. All the components that are used in the virtual experiment are discussed. A description of the device is presented. The results of the virtual experiment will be discussed.

1. Introduction

Mcstats is a Neutron scattering ray-tracing simulation tool which uses the Monte-Carlo method. The Monte-Carlo method can be defined simply as an application of the law of large numbers. The Monte-Carlo computer techniques require that the random numbers be unbiased independent variables. The choice of the random number generator is essential to ensure a proper estimate consistency, and the development of the Monte-Carlo techniques have triggered much effort in the computational, pseudo-random number generator algorithms, such as the well known linear congruential generator (using modulus). One way to quantify the efficiency of these random number generators resides in their periodicity, that is the maximum pseudo-random sequence length before it repeats itself, and their maximum dimensionality, that is the maximum sequence length that can be thrown and considered to hold independent equidistributed numbers.[1]

Mcstats is used to do virtual experiment which in the
end help to understand the instrument pitfalls and improve their usage.

We can define a neutron scattering Virtual Experiment as a simulation in which:

1. models a complete instrument, including a detailed sample description,
2. provides absolute intensity results that compare with actual measurements, and
3. can be controlled like a real instrument.

The key point in these requirements is certainly the availability of advanced and accurate sample and neutron optics descriptions.

Compared with other neutron propagation Monte-Carlo codes, the Mcstas package has put much effort in these fields and achieved a significant breakthrough towards effective Virtual Experiments, for all classes of neutron scattering instruments and materials. [1]

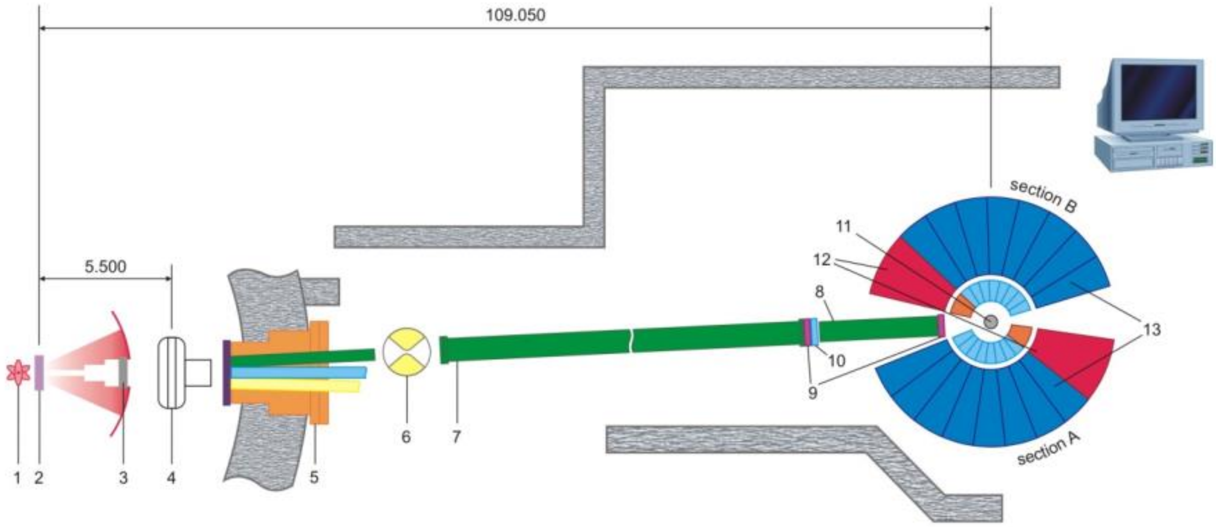

Figure 1 he layout of the NERA spectrometer: 1 – IBR-2 reactor core, 2 – thermal and cold moderators of radial horizontal channels 7-11 and tangential channels 1–9, 3 – beam shutter, 4 – fast neutron background chopper, 5 – common vacuum splitter of three Ni-mirrors neutron guides, 6 – λ- chopper of beam 7b, 7 – vacuum Ni–mirrors guide tube of neutron beam 7b, 8 – vacuum sections of beam 7b, 9 - diaphragms of incident beam, 10 –monitor, 11 – sample position, 12 – NPD sections, 13– INS and QENS sections. [2]

NERA is an indirect geometry spectrometer designated predominantly for the study of molecular dynamics. The instrument is located at a distance of 100 m from the ambient water moderator at the end of the neutron guide. NERA can also be used as a diffractometer; the range of detected scattering angles provides good resolution in the Q-range (0.7 – 21 Å-1). The sample environment system on NERA permits inelastic and diffraction experiments at low temperatures (5K-300K) and high pressures up to 400 MPa.

The scientific program on NERA includes studies of hydrogen-bonded systems, biologically active materials, organic compounds; study of properties of dynamic complexes with transfer of electric charge, etc. [2]

I. Neutron source

There are different ways to differentiate between neutron sources types.

We can differentiate between neutron sources types by the origin of producing neutrons. In this case there are two common ways which are the neutron source can be a nuclear reactor or a spallation source.

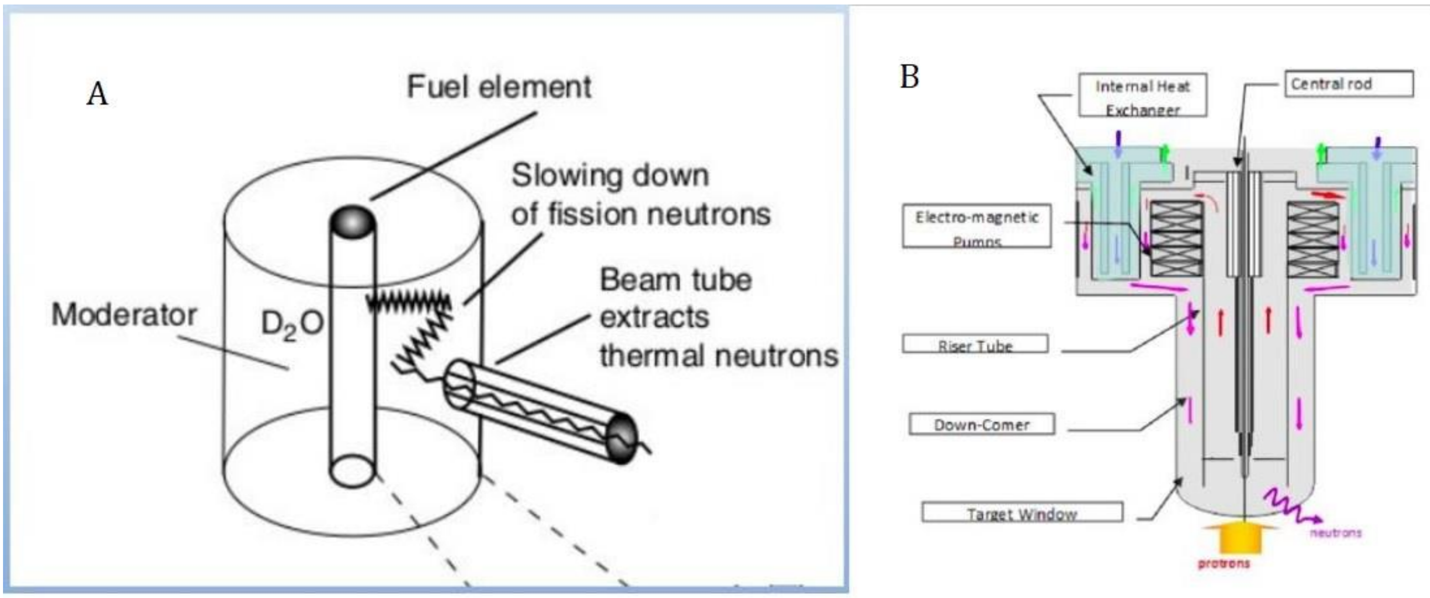

Figure 2. (a) simplified nuclear reactor showing how we can extract neutrons (b) simplified spallation source

In the case of a nuclear reactor, the neutron flux is withdrawn from the core. The spallation source is configured with a particle (proton) accelerator. As a result of the collision with a metal (Pb, Hg, W) target, protons initiate nuclear transformation –spallation.

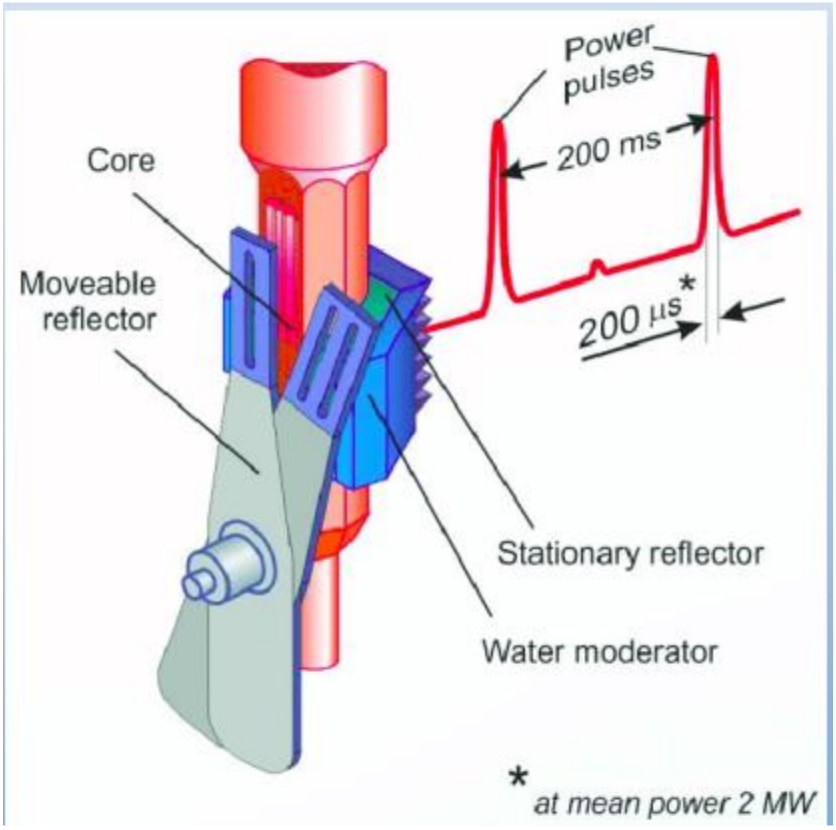

Figure 3. Pulsed neutron source.

The neutron sources can also be divided into a continuous or a pulsed source of neutrons according to their time characteristics.

The advantage of pulsed sources is the ability to determine the neutron energy from the time of flight. Pulsed sources only make sense if one can make effective use of theflux in each pulse, rather than the average neutron flux.

The energy spectrum of neutrons coming straight from the source usually does not correspond to the energyrange that is useful in studying the structure and dynamics of solids.

In order to lower the average energy of neutrons in the stream moderators, are used. They are usually materials with a high content of hydrogen atoms (protium or deuterium), e.g. heavy water, aromatic hydrocarbons at low temperatures.

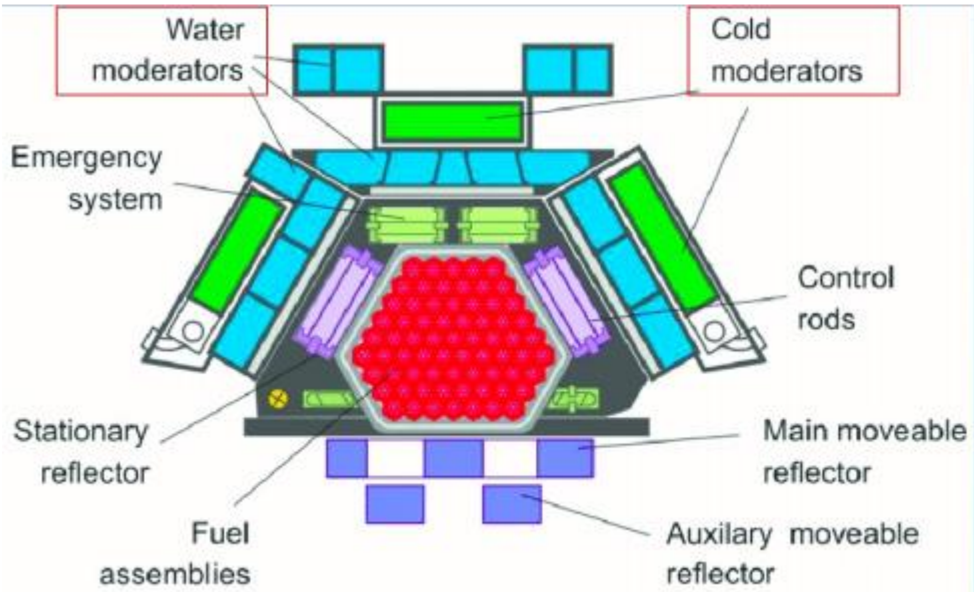

Figure 4. IBR-2 plused reactor

The IBR-2 reactor with its unique technical approach produces one of the most intense neutron fluxes at the moderator surface among the world's reactors: $\sim10^{16}$ n/cm^2/s, with a power of 1850 MW in pulse. The reactor operates continuously for a 12 day cycle followed by a shutdown to prepare for the next experiments. In addition, there is a longer shutdown to carry out necessary maintenance work during the summer time. Normally there are about 9 cycles a year.[3]

II. Neutron guides

Figure 5. Straight rectangular guide.

Main task of neutron guides is to transport neutrons without a loss of flux. Neutron guides might me also curved in a way, that prevents the fast neutrons from reaching sample position. Other properties of neutron guides may be, for example, focusing the beam. This is done by curving the guide’s profile.

Figure 6. Long replica tube.

Long replica tube is a guide for ultracold neutrons is made by using a polished glass plate was coated with a nickel layer, reinforced with a galvanised nickel layer and removed from the glass. Then rolled to a tube and welded.

III. Choppers

Choppers are rotating discs with a slot with an appropriate geometry. The selection of the desired wavelength can also be made on the basis of a time-of-flight calculation. This is the job of velocity selectors or components called choppers.

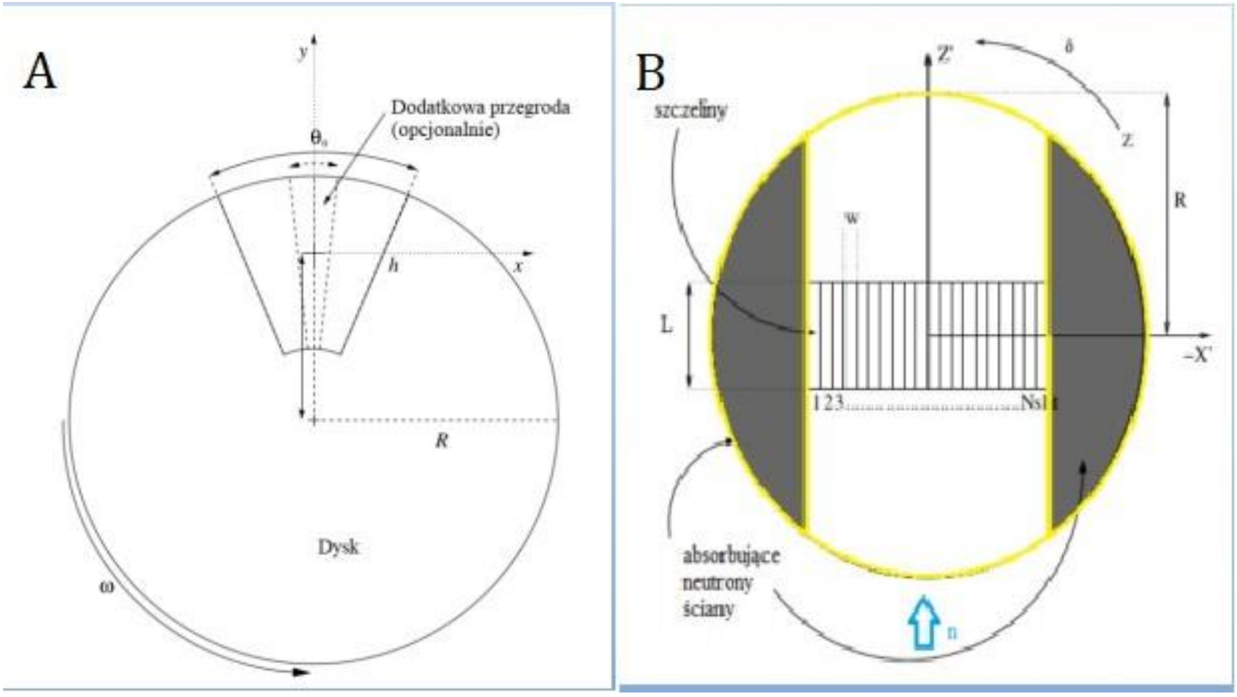

Figure 7 (a) Disc chopper (b) Fermi choppers

The chopper's axis of rotation can be horizontal - then it is called Disc chopper. In the case of a disc chopper, the most common is a single channel / slot that is not curved and its shape is a quadrangle or a segment of a circle. Fermi choppers have a vertical axis of rotation. The Fermi chopper has many smaller channels located along the diameter of the disc.

IV. Monochromators/ Analyzers

Monochromators and analyzers are instrument components that extract a fraction of the desired wavelength (energy) from the polychromatic neutron beam. Selection of a given wavelength (neutron energy) is done using Bragg's law.

Figure 8. Focusing monochromator unit

Monochromators that are crystals (crystalline bodies) with some exact d-spacing. Appropriate setting of the crystal or
crystal matrix on the way of a polychromatic neutron beam causes
their scattering according to the rule described by Bragg's law. If it is in front of the sample, we call it a monochromator, if it is between the sample and the detector, we call it the analyzer.

2. Description of the device

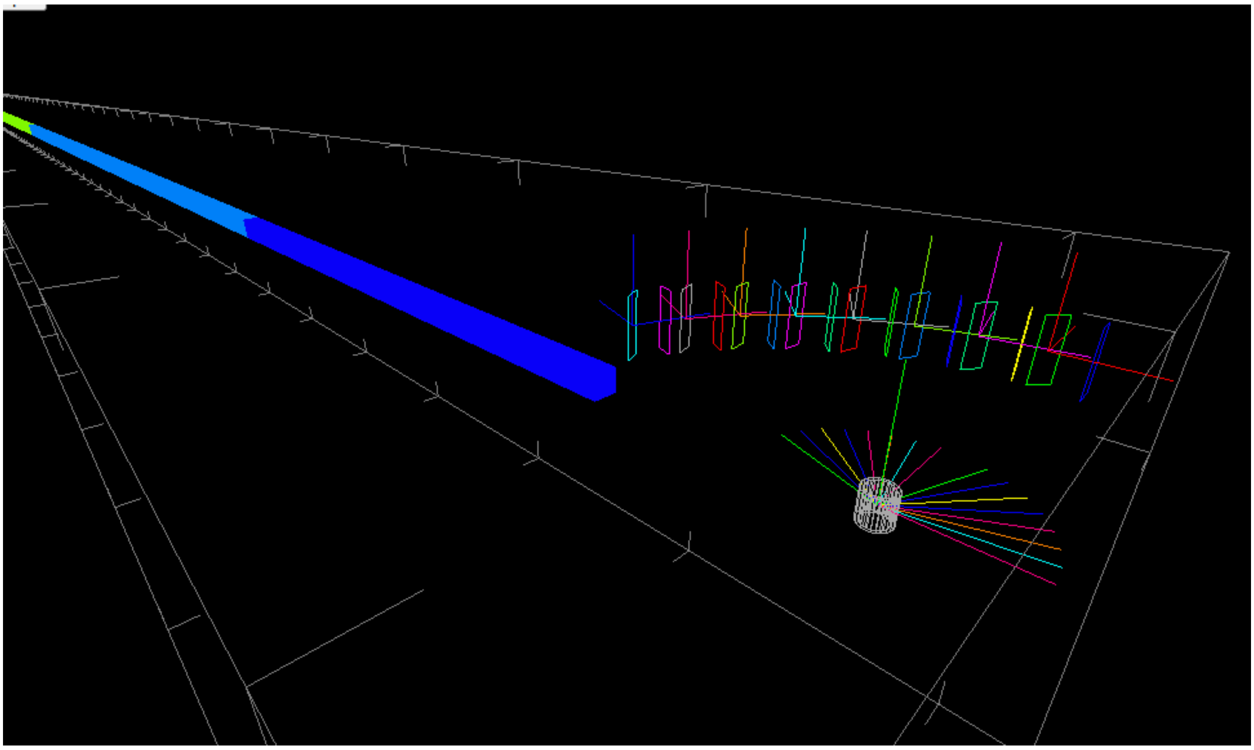

Figure 9. The sample surrounded by analyzers and moniters

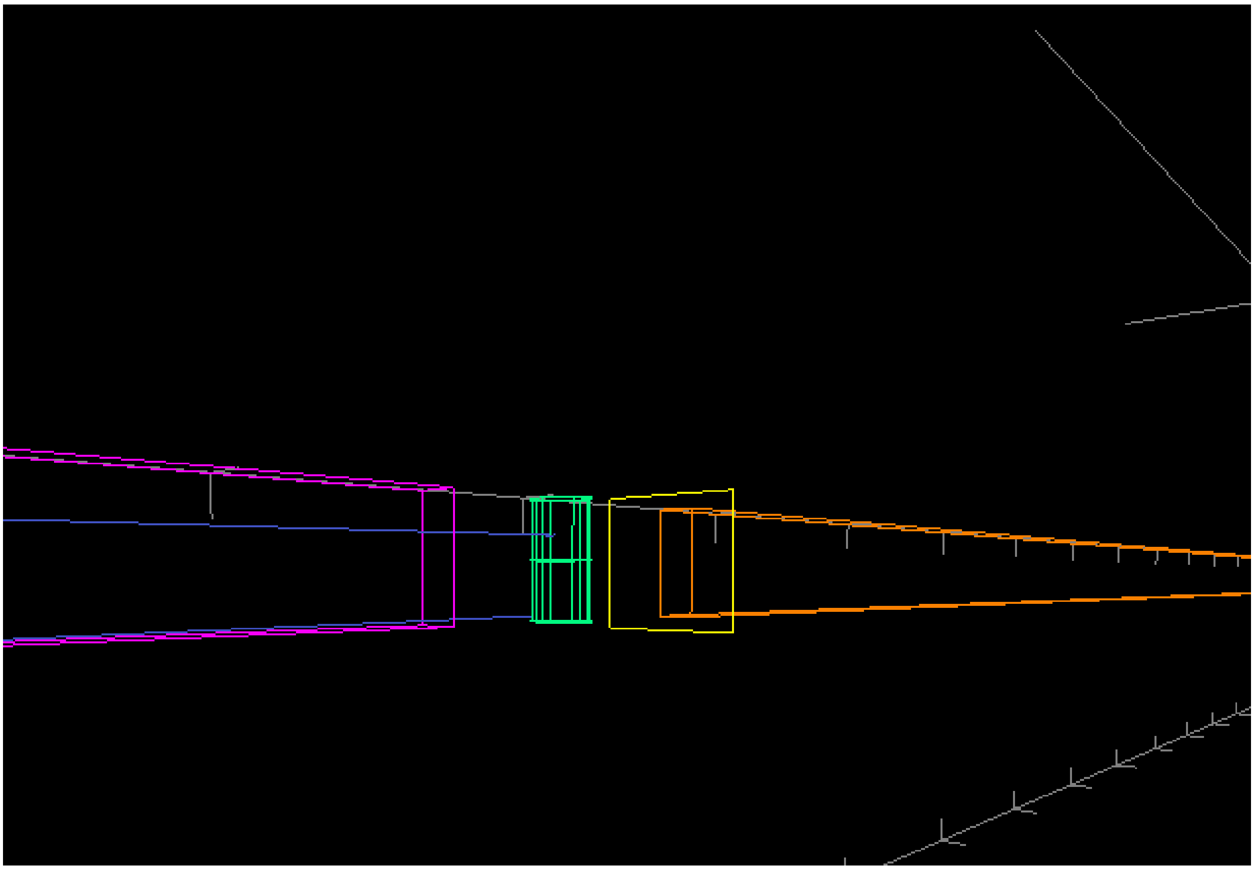

Figure 10. The Fermi Chopper

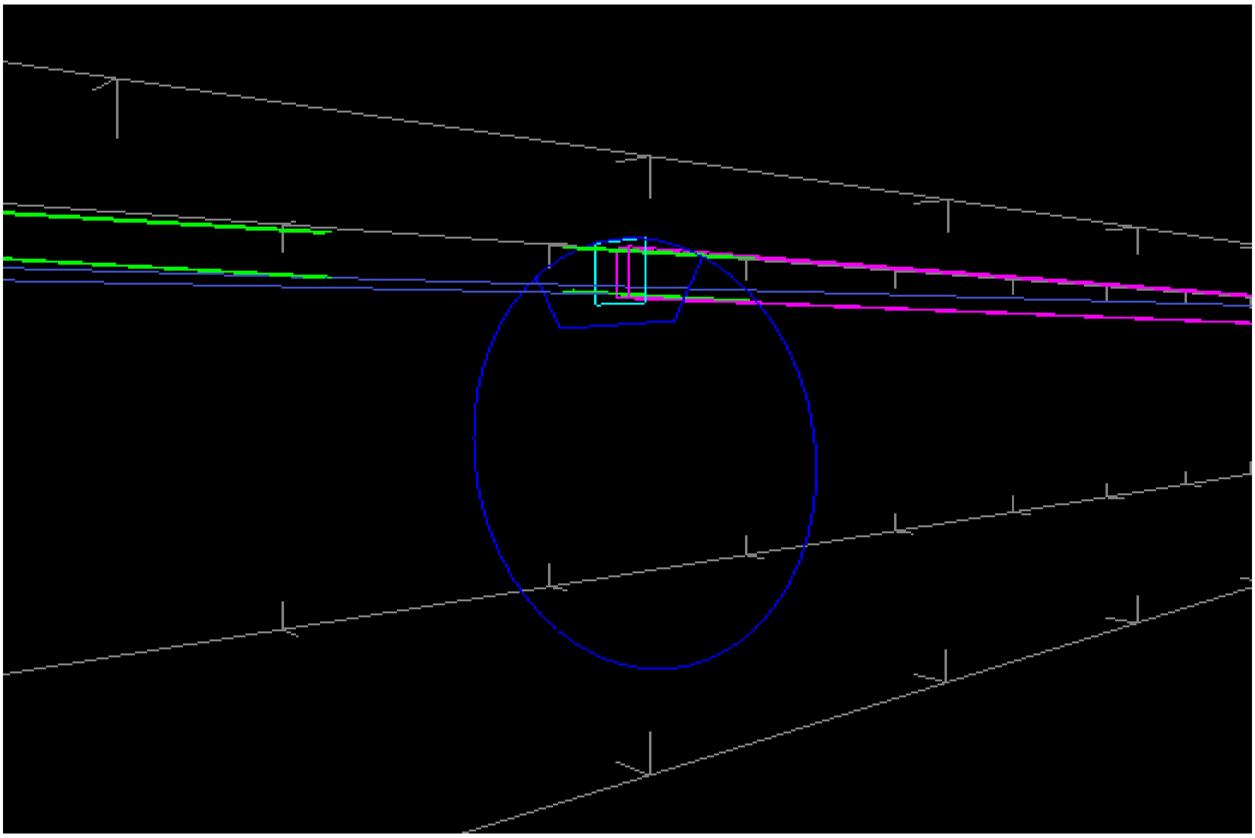

Figure 11. The Disk Chopper

The virtual experiment starts with a continous source unlike in NERA which depends on the IBR-2 plused reactor. The neutron energy is distributed in wavelength between 0.1 and 20 angstrom. The source length is 6 meters.
The next componant is a fast rotating disc with the rotating axis parallel to the neutron beam. The disk chopper is used to cut a continuous neutron beam into short pulses. The disk consists of neutron absorbing materials. To form the pulses the disk has openings through which the neutrons can pass. The disk chopper has a delay of 0.001 s. The disk chopper is connected to a Fermi chopper with a simple rectangle guide. The guide is centered on the z axis with rectangular entrance and exit openings parallel to the x-yplane.
The Fermi chopper is a rotating vertical cylinder containing a set of collimating slits. The Fermi chopper in this virtual experiment consist of only one slit just like in NERA. The sample which is used vanadium, because vanadium gives an isotropic, elastically scattered beam.
The sample is designed to only have absorption and incoherent elastic scattering. The incoherent scattering gives a uniform angular distribution of the scattered neutrons from each nucleus. The radius is 0.025 m and the thickness is 0.005 m. The sample is surrounded by analyzers which are on a perimeter of an upper half circle.There are 8 each one is rotated with a bragg angle of 45 degrees relative to the sample.

3. Results Discussion

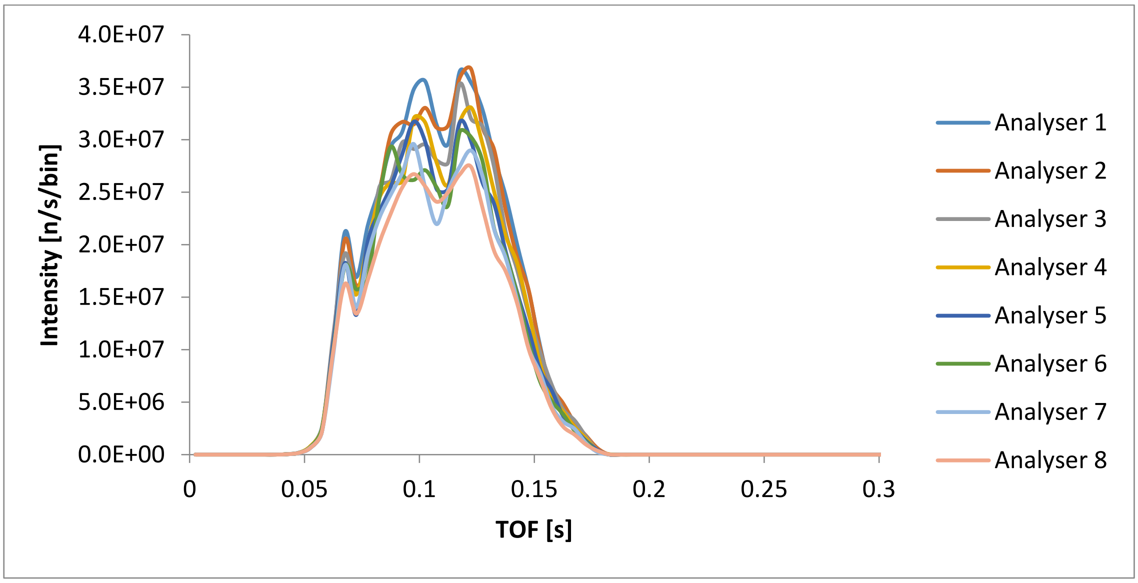

Figure 9.Time distribution from the Analyzers surrounding the sample.
The TOF incident neutron spectra measured from detectors after the analyzers. The TOF scale can be easily transformed to the neutron wavelength scale using the following relation.

$$\lambda = h/mv \text{ or } \lambda[\text{Å}] = 3.956 \times 10^{-3}\ t\,[\mu s]/\ L[\text{m}],$$

where: h is Planck's constant, λ, m and v are the neutron wavelength, mass and velocity respetively. t is the time of flight and L – is the average total distance from the source to the detectors. The different shapes are a result of the neutron beam reaching the sample position suffers a number of artefacts. In particular, the neutron energy and pulse length defined by the choppers are not perfect, so that it also broadens the time axis on the detector.[1,4] And, as the neutron beam is not strictly parallel, a distribution of incoming neutron momentum directions will result in a broadening of the angular axis. Finally, a variation of the time of flight originates from the sample volume itself which introduces an additional path length to travel to the detector. All of these effects are common on all neutron scattering instruments and may be analyzed and corrected. But the addition of all imperfections may not be easily corrected, as they are usually cross-correlated. The more complex the instrument is, the more measurement artefacts appear, and the harder it is to apply simple analytic corrections. [6]

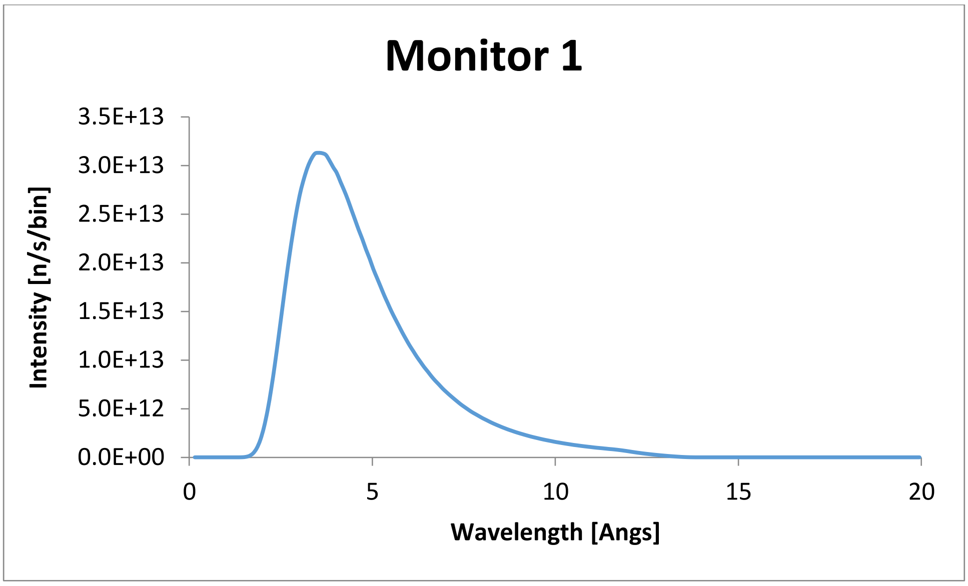

Figure 10. The wavelength distribution around λ = 3.3 Å obtained after the diskchopper

Incident neutrons spectra after the diskchopper Fig. 10 has a wavelength distribution around = 3.3 Å which is close to the experimental results in [5] Figure 6. From Figure we can notice that the Intensity closes to zero after λ= 14 Å wavelengths. The maximum neutron intensity is 3.13×10^{13} which corresponds to λ 3.5 Å.

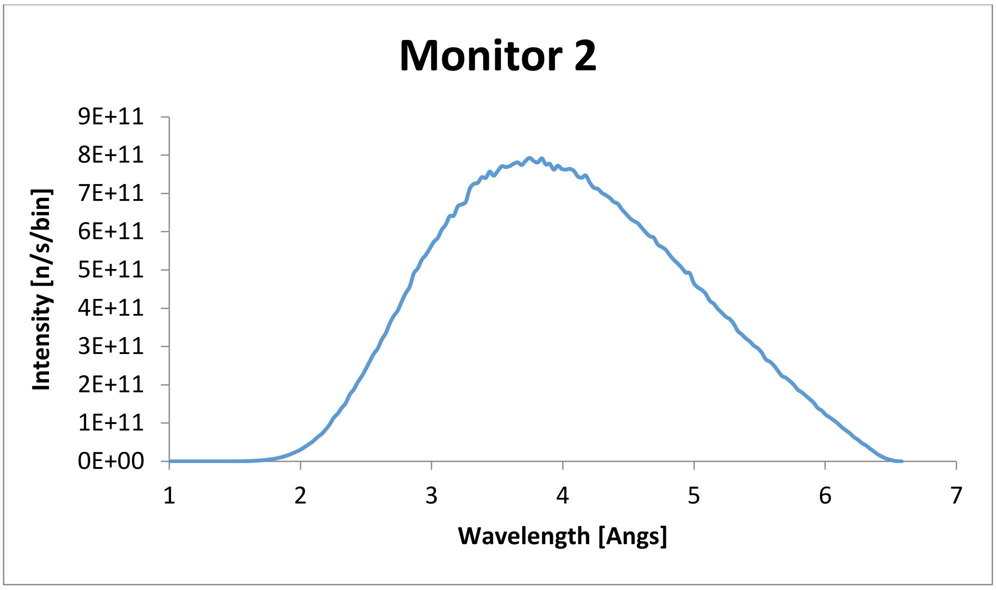

Figure 11. The wavelength distribution around λ = 3.7 Å obtained after fermi chopper

The Fermi chopper wavelength resolution will get narrower as the frequency increases and the slit width decreases, which also leads to a decrease in intensity. From the Fig. 11 we find the higest neutron intensity per bin is around 7.93×10^{11} which corrsponds to a wavelength distribution around λ = 3.7 Å. The wave length obtaind is a few percent around the central transmitted wavelength.

4. Acknowledgement

I'm very grateful to Marta Klepacka for her detailed explanation of every part of Mcstats and her dedication for teaching by preparing a strong introductory material for Mcstats, and also her assignments which deepened my understanding of the material. I would also like to thank JINR for this wonderful opportunity to provide a world-class education for free and their wonderful support team for their fast and instructive response. I was honored to participate in the INTEREST program, and I will be honored if I can participate in any JINR programs in the future.

5. References

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