**Monte-Carlo simulation of neutron scattering experiment**

Frank Laboratory of Neutron Physics

MSc Marta Klepacka

***Abstract:***

The main goal of the practice is to learn the neutron scattering simulation software McStas. McStas has been a successful tool for designing and optimizing neutron instruments for over 20 years now and it is still upgrading, allowing even more advanced analysis of designed neutron scattering instruments.

Two key elements of McStas software are Monte-Carlo algorithms and ray-tracing. Thanks to Monte-Carlo implementation, simulating very complex physical phenomena as neutron scattering is possible with a great accuracy. Ray-tracing allows the designer to approximate the most probable paths of neutrons inside the neutron scattering instrument. With McStas tools an extended analysis of designed instrument can be done, for example: measuring beam divergence at any point in instrument, measuring wavelength and energy spectrum of a beam, plotting 2D and 3D graphs for chosen parameters in space and time, calculating the spectrometer resolution and many more.

***Tasks***

1. Choosing and calculating neutron scattering experiment setup parameters.

2. Learning the McStas software.

3. Understanding and applying Monte-Carlo methods.

4. Designing neutron scattering instruments in McStas (TAS and ToF spectrometers).

5. Optimizing instrument’s components according to the goal of experiment.

***Preliminary schedule by topics/tasks:***

The duration of this project is 5 weeks.

***1st & 2nd week***: Introductory talks:

* Neutron scattering theory.
* Neutron scattering instrumentation.
* Monte-Carlo methods.
* Experimental setups for neutron scattering.
* Introduction to McStas software.

***3rd week:***

* Designing TAS and ToF instruments in McStas.

***4th week:***

* Optimization of designed instruments.
* Running scans in McStas.

***5th week***: Preparation and writing a report

***Required skills:***

1. Basic knowledge of condensed matter physics.

2. Principles of neutron scattering.

3. Basics of Monte-Carlo methods.

4. Programming (C++) skills are not necessary for McStas beginners. However, they would be a significant advantage to start with.

***Acquired skills and experience:***

1. Understanding Monte-Carlo simulations characteristics.
2. McStas software skills.
3. Designing and optimizing a neutron scattering experiment.

***Recommended literature:***

1. Schober H., Neutron Scattering Instrumentation. In: Liang L., Rinaldi R., Schober H. (eds) Neutron Applications in Earth, Energy and Environmental Sciences. Neutron Scattering Applications and Techniques. Springer, Boston, MA, 2009, https://doi.org/10.1007/978-0-387-09416-8\_3

2. R. Pynn, Neutron scattering: a primer, Los Alamos Science, 1990

3. Farhi E., Willendrup P., Virtual experiments in a nutshell: Simulating neutron scattering from materials within instruments with McStas, EDP Sciences, 2011,
DOI: 10.1051/sfn/201112015